Preparati protiv ispadanja kose : sastav i mogući utjecaj na zdravlje

Jović, Ines

SVEUČILIŠTE U SPLITU
MEDICINSKI FAKULTET

INES JOVIĆ

PREPARATI PROTIV ISPADANJA KOSE: SASTAV I MOGUĆI UTJECAJ NA ZDRAVLJE

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Prof.dr.sc. Davorka Sutlović

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Mentor: prof.dr.sc. Davorka Sutlović

PREPARATI PROTIV ISPADANJA KOSE: SASTAV I MOGUĆI UTJECAJ NA ZDRAVLJE

Ines Jović, broj indexa 204

Sažetak:

Ciljevi istraživanja: Kvalitativnom metodom (GC-MS) odrediti sastav preparata protiv ispadanja kose te usporediti navode deklaracija s dobivenim rezultatima.
Ustroj istraživanja: eksperimentalna studija
Materijali i metode: Ispitana su 2 uzorka preparata protiv ispadanja kose. Za pripremu uzorka korištene su staklene Petrijeve zdjelice na koje je nanesen uzorak volumena 100 μL. Uzorci su ekstrahirani smjesom organskih otapala, kloroforma, etil acetata i N-heksana u jednakom omjeru (v/v/v= 1:1:1), te su potom postavljeni u digestor na sušenje u struji zraka. Kromatografska analiza pripremljenih ekstrakata izvedena je na plinskom kromatografu sa spektrometrom masa, metodom koja omogućava istovremeno snimanje ukupnog ionskog kromatograma (*engl. Total ion chromatogram*, TIC) u području od 40 – 600 m/z i snimanje samo odabranih iona (*engl. Single ion monitoring*, SIM).
Rezultati: Kvalitativnom analizom uzoraka dobili smo rezultate koji su izlistani u analitičkom izvješću. U prvom uzorku su pronađene tvari koje nisu navedene među pomoćnim tvarima, ali prema visini signala možemo zaključiti da se radi o tvarima koje se nalaze u tragovima. U trećem uzorku nismo pronašli sve tvari koje proizvođač navodi na ambalaži, a kofein koji je jedan od sastojaka je pokazao jako visok signal što odgovara visokoj koncentraciji.
Zaključak: Ovim istraživanjem je provedena samo kvalitativna analiza te bi za detaljniju obradu dobivenih podataka trebalo provesti i kvantitativnu analizu kako bi u potpunosti točno interpretirali rezultate.

Ključne riječi: kosa, rast, GC-MS metoda
Rad sadrži: 65 stranica, 11 slika, 48 literaturnih referenci
Jezik izvornika: hrvatski

Sastav povjerenstva za obranu:
1. prof.dr.sc. Ivana Mundić predsjednik povjerenstva
2. prof.dr.sc. Neira Puizina Ivić član
3. prof.dr.sc. Davorka Sutlović mentor

Datum obrane: rujan 2021.

BASIC DOCUMENTATION CARD

GRADUATE THEISS

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Mentor:	Davorka Sutlović, PhD, full prof.

ANTI-HAIR LOSS PRODUCTS: COMPOSITIONS AND POSSIBLE HEALTH IMPACT

Ines Jović, 204

Summary:

Objectives: Qualitative determination of ingredients in products for hair loss using GC-MS method, as well as the comparison of the results with those declared on the product.
Design: Experimental study
Material and Methods: Two samples of anti-hair loss products were tested. Petri dishes were used to prepare the sample and volume of 100 μL was applied. Samples were extraced with a mixture of organic solvents, chloroform, ethyl acetate and N-hexane in equal ratio (v / v / v = 1: 1: 1), and then placed in a digester to air dry. Chromatographic analysis of the prepared extracts was performed on a gas chromatograph with a mass spectrometer, a method that allows simultaneous recording of the total ion chromatogram (TIC) in the range of 40 - 600 m / z and recording only selected ions (single ion monitoring, SIM).
Results: By qualitative analysis of the samples, we obtained the results listed in the analytical report. In the first sample, substances were found that are not listed among the excipients, but according to the signal height, we can conclude that these are trace substances. In the third sample, we did not find all the substances listed by the manufacturer on the packaging, and caffeine, which is one of the ingredients, showed a very high signal, which corresponds to a high concentration.
Conclusion: With this research, only a qualitative analysis was performed, and for a more detailed processing of the obtained data, a quantitative analysis should be performed in order to fully interpret the results.

Keywords: hair, growth, GC-MS method
Theiss contains: 65 paiges, 11 figures, 48 references
Original in: Croatian

Defence committee:
1. Ivana Mundić PhD full prof. chair person
2. Neira Puizina Ivić PhD full prof. member
3. Davorka Sutlović PhD full prof. supervisor

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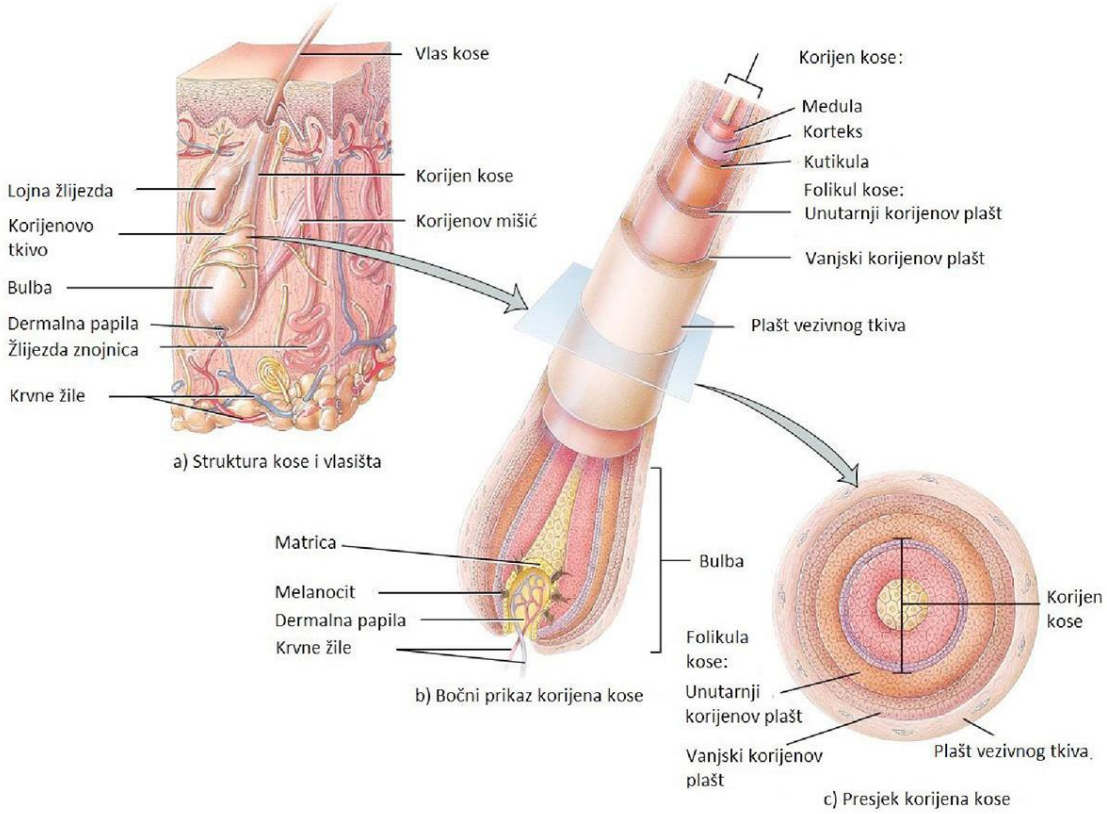
Sadržaj

1. UVOD

Današnje društvo stavlja velik naglasak na vanjski izgled, a kosa je vrlo važna komponenta cjelokupne slike. Kosa predstavlja bitan dio ljudskog tijela i jedan od glavnih modnih detalja te predstavlja statusni simbol kroz cijelu povijest pa sve do danas. U antičko doba dlake su bile poznate kao zaštitni pokrivač te se po količini, vrsti i boji kose moglo prosuditi kojem se društvu pripada. (1) Gubitak kose predstavlja manji zdravstveni problem gledajući pacijentovo fizičko zdravlje međutim za njih je uznemirujuć i značajno utječe na kvalitetu života. (2) Pacijenti imaju osjećaj manje vrijednosti te istraživanja pokazuju kako osobe s alopecijom imaju veću incidenciju psihijatrijskih poremećaja kao što je socijalna fobija, anksioznost pa i depresija u usporedbi s ostatkom populacije, a posebice je izraženo kod žena. (3) Gubitak kose je stanje koje ima značajne implikacije za psihosocijalne funkcije pacijenata te im se izmjenjuju osjećaji tuge, bijesa, srama i nelagode. (4) Kosa je primarna karakteristika sisavaca te ima širok raspon funkcija kao što je termoregulacija, fizička zaštita i osjetna aktivnost. (5) Ima senzornu funkciju proširujući osjet dodira koji se javlja na razini kože. Kosa s vremenom može modificirati svoju boju, od dlačica velusa kod beba (neobojena,meka kosa) do konačne dlake odraslih muškaraca (obojena brada,gusta i jaka kosa). Starenjem kosa gubi svoj pigment te postaje bijela. Također štiti vlasište od štetnog ultraljubičastog zračenja te djeluje kao krema za sunčanje. (3) Problem gubitka kose pogađa muškarce i žene, a s obzirom da uzroci mogu biti mnogobrojni predstavlja velik izazov za liječnike kako bi pronašli uzrok, ali i učinkovito rješenje tog problema. Različiti čimbenici mogu dovesti do kliničkog gubitka kose ili alopecije, uključujući genetsku predispoziciju, lijekove, sistemske bolesti, traumu, prehranu, endokrine i psihološke abnormalnosti. Upravo zbog tih mnogobrojnih smetnji koje mogu rezultirati gubitkom kose važno je napraviti temeljit fizikalni pregled i uzeti anamnezu. Za potvrdu dijagnoze ponekad je potrebna pomoćna labaratorijska procjena. (6)

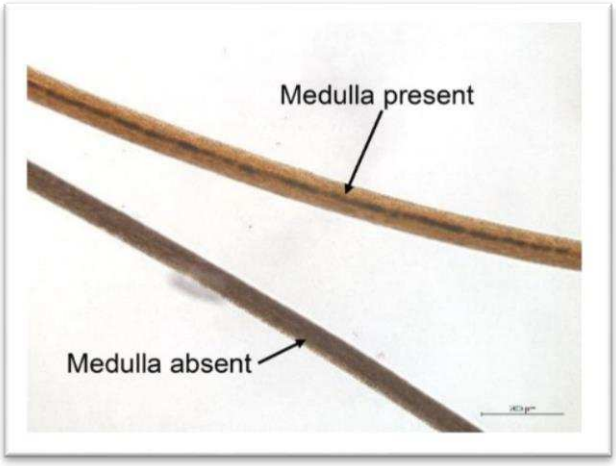
1.1. Građa dlake

Kosa može rasti pojedinačno, u skupinama od dva do tri ili ponekad u skupinama od četiri do pet, a te skupine su poznate kao folikularne jedinice. (7) Kosa se sastoji od dva dijela : folikula u koži i vlasi koja je vidljiva na površini tijela. Folikul je podijeljen u tri dijela.



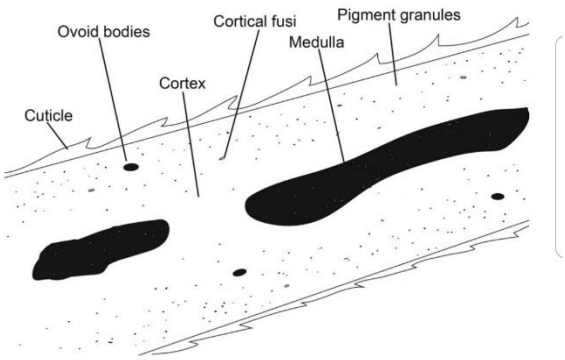
Slika 1. Struktura kose i vlasišta (8)

Gornji dio je infundibulum i proteže se od ulaza u folikul do mjesta gdje se ulijeva sekret žlijezde lojnice. Isthmus predstavlja srednji dio i proteže se od uljeva žlijezde lojnice do hvatišta koštrijenog mišića. Preostali dio je inferiorni segment. (1) Korijen dlake ima proširenu glavicu poput lukovice te je tu utisnuta papila gdje se nalazi mreža krvnih žila čija je uloga opskrba hranjivim tvarima te se na taj način potpomaže rast kose. (9) Vlas kose je podijeljena u tri segmenta. Medula (moždina) predstavlja sredinu kose te je većina dlaka ne sadrži dok kod onih koje ju imaju je fragmentirana ili isprekidana, a ovaj sloj posebno nedostaje sitnim dlačicama. (1) One koje sadrže medulu imaju glikogen vakuole i medularne granule koje sadrže citrulin. (7)



Slika 2. Prikaz medule (10)

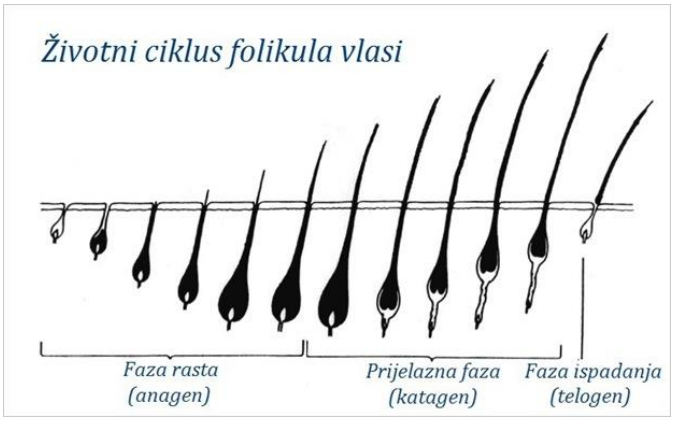
Sljedeći segment je korteks (kora) koji čini najveći dio dlake,a glavna uloga je da daje mehaničku čvrstoću. Sastoji se od visoko strukturiranog proteina, keratina, a čine ga duge spiralne niti. Nitaska struktura je odgovorna za pružanje otpora dok spiralna daje elastičnost. (7) Aminokiseline u keratinu su povezane s različitim kemijskim vezama. Disulfidna veza se nalazi u cisteinu i poprečno povezuje lance keratina , a njihov broj ovisi o vrsti kose. Kosa koja sadrži više tih veza otpornija je na kemikalije i mehaničku obradu. Amidna veza je odgovorna za povezivanje aminokiselina u spirale polipeptidnih lanaca koji su dugi kao vlas. Vodikovi mostovi uspostavljaju vezu između imidne i karbonilne skupine u suhoj kosi. Ionska veza povezuje amino te karboksilne skupine dok hidrofobna povezuje postrane lance u molekulama aminokiselina. (9) Kora pohranjuje većinu vlažnosti kose te joj osigurava boju. Broj, distribucija i vrste granula melanina sadržane u kori su ono što vlaknima dlake daje pigment. (7) Vanjski sloj vlasi čini kutikula. (1) Sastoji se od pet do deset preklapajućih keratiniziranih stanica koje se međusobno pokrivaju poput krova. (9)



Slika 3. Prikaz dijagrama mikrostrukture kose (10)

1.2. Faze rasta dlake

Svaka vrsta kose prolazi ponovljeni ciklus aktivnog rasta i odmora, a trajanje svakog ciklusa se razlikuje među pojedincima. (1) Prosječan čovjek ima oko 100 000 vlasi kose, svaka u različitim stupnjevima ciklusa rasta dlake. Postoje tri glavne faze rasta dlake: anagena (faza rasta), katagena (prijelazna faza) i telogena (faza mirovanja). Anagena faza u prosjeku traje od dvije do sedam godina, katagena približno dva tjedna, a telogena oko tri mjeseca. U anagenoj fazi se nalazi oko 84% vlasišta, u katagenoj 1 do 2 % dok je u telogenoj oko 10 do 15%. (7) Anagena faza je stadij u kojem dolazi do intenzivne mitotičke diobe u području matriksa vlasi te orožnjavanja i oblikovanja složene valjkaste tvorbe koja stalno raste. Tijekom te faze dlaka nikada ne ispada spontano, a prilikom čupanja se osijeća bol. (9) Anagena faza je stadij aktivnog rasta u kojem folikul doseže maksimalnu duljinu i volumen. (7) Katagen se odnosi na razdoblje involucije. (7) U toj fazi stanice se podvrgavaju apoptozi i kosa prestaje rasti te dolazi do uvlačenja folikula. (10) Telogena faza predstavlja uspavani stadij u kojem dolazi do izrazitog smanjenja proliferacije i biokemijske aktivnosti folikula dlake. Tijekom ove faze estrogenski receptori su maksimalno izraženi. (7) Novi ciklus slijeda anagen-katgen-telogen je iniciran s neomorfogenezom, procesom koji se naziva neogen. Do toga dolazi kada se dermalna papila ponovno poveže s matičnim stanicama generirajući novu dlaku. (10)



Slika 4. Životni ciklus folikula vlasi (9)

1.3. Uzroci gubitka kose

1.3.1. Telogeni efluvij je jedan od najčešćih uzroka alopecije. (11) To je oblik alopecije bez ožiljaka koju karakterizira difuzno, često akutno ispadanje kose. (12) Čimbenici kao što je traumatčan događaj, fiziološki i emocionalni stres mogu dovesti do toga. (11) Brojni lijekovi

se povezuju s ovim stanjem kao što su beta blokatori, retinoidi, antikoagulansi, propiltiouracil te karbamazepin. (12) Postoje brojne hipoteze koje opisuju patofiziologiju telogenskog efluvija. Neke od njih su: trenutačno oslobađanje anagena gdje folikuli napuštaju fazu anagena te prerano ulaze u fazu telogena, a to dovodi do povećanog osipanja dva do tri mjeseca kasnije. Zatim odgođeno oslobađanje anagena u kojem je anageni stadij produljen te dolazi do teškog otpadanja u telogenu. U sindromu kratkog anagena kao posljedica idiopatskog skraćivanja anagena dolazi do postojanog telogenskog efluvija. Kod trenutačnog oslobađanja telogena skraćena je telogena faza pa dolazi do masovnog oslobađanja dlaka. Postoji i odgođeno oslobađanje telogena u kojem je produžena telogena faza, a odgođen prijelaz u fazu anagena. (11)

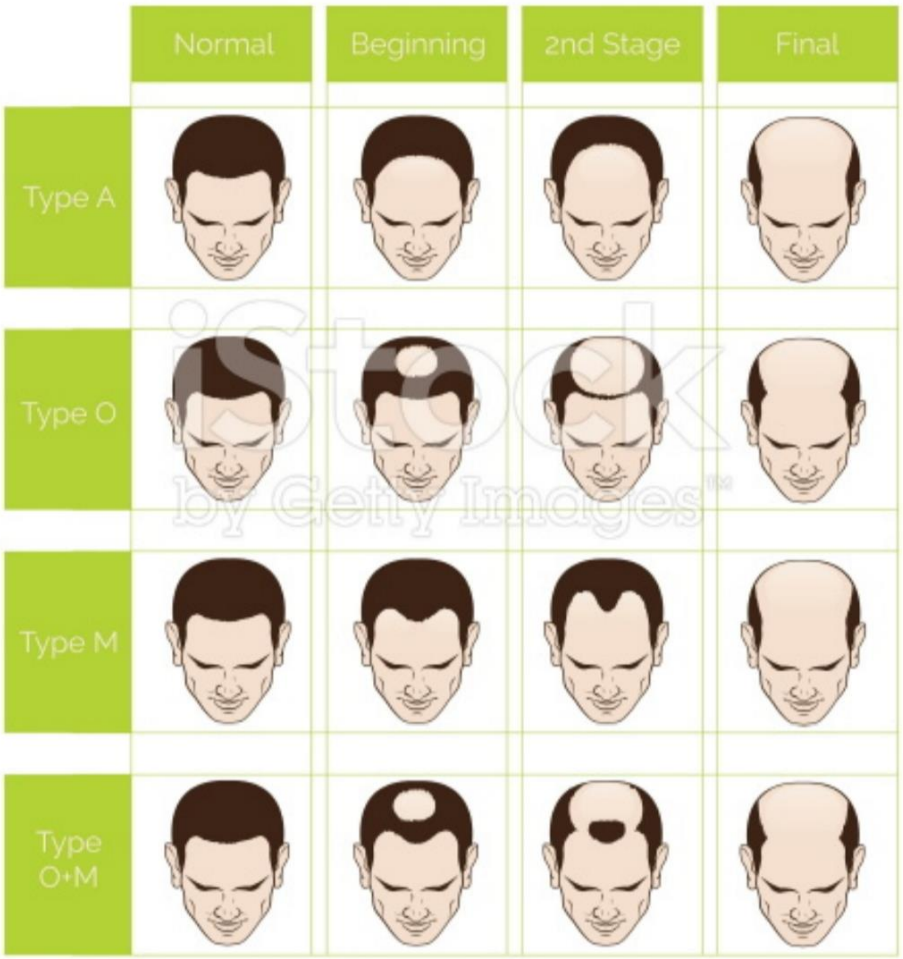
1.3.2. Prehrana

Prehrana je ključna u održavanju zdrave kose, a posebno važni su proteini kao što je keratin koji čini primarnu komponentu kose. (4) Kod pacijenata s Kwashiorkom ili anoreksijom neadekvatan unos proteina povezuje se s nedostatkom kose. (3) Razina vitamina D, cinka i folata u serumu se pokazala nižom kod pacijenata koji boluju od alopecie areata u odnosu na kontrolu međutim dosadašnja istraživanja su nedostatna kako bi se suplementacija mikroelementima mogla koristiti kao metoda liječenja. (13) Prekomjerna razina vitamina A također može dovesti do gubitka kose. Određene studije pokazuju povezanost između nedostatka željeza i alopecije te su određene ustanove zauzele stav da se gubitak kose poboljšava liječenjem tog nedostatka međutim potrebni su konačni dokazi koji bi mogli potvrditi učinkovitost tog liječenja. (4)

1.3.3. Endrokrina neravnoteža

Muški obrasci gubitka kose su vrlo često povezani s hiperandrogenemijom, ali kod žena je ta veza nešto slabija. (4) Muška androgena alopecija predstavlja najčešći oblik gubitka kose kod muškaraca, a koji pogađa 30-50% muške populacije do 50.godine života. (14) Oko 38% žena koje imaju problem gubitka kose imaju i povišenu razinu androgena. (4) Ključne patofiziološke značajke ovog stanja su promjena u razvoju ciklusa dlake te upala. Duljina anagena se sa svakim ciklusom smanjuje dok telogena faza ostaje konstantna ili se produljuje dok u konačnici anagena faza postane toliko kratka da kosa koja raste ne može postići dovoljnu dužinu da dosegne površinu kose. (14) Poremećaji rada štitnjače obuhvaćajući hipertireozu kao i hipotireozu mogu dovesti do alopecije. (4) Pojedini slučajevi prikazuju pacijente koji su se

borili s gubitkom kose te im je pravilnom dijagnozom Hashimotovog tiroiditisa određena terapija levotiroksinom te se gubitak kose nakon određenog vremena riješio. (15)

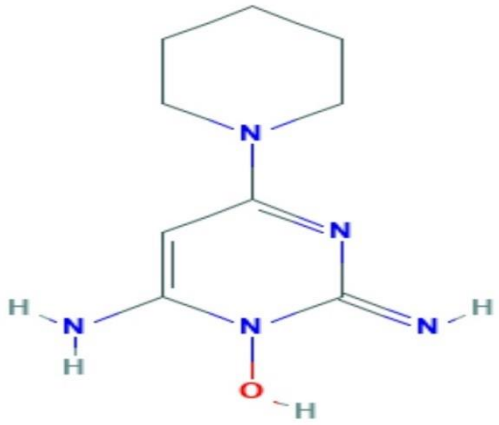


Slika 5. Faze ispadanja kose (16)

1.4. Odobreni lijekovi

Američka agencija za hranu i lijekove (*Food and Drug administration*, FDA) je odobrila lokalni minoksidil i oralni finasterid za liječenje muške androgene alopecije. Oba lijeka će spriječiti daljnu ćelavost, ali djelomično te zahtjevaju kontinuiranu upotrebu kako bi se učinak održao. (14) Minoksidil je zapravo izravni vazodilatator koji je uveden 1970-ih za liječenje hipertenzije. Njegova istaknuta nuspojava je hipertrihoza koja je ograničavala upotrebu posebice kod žena. (17) Njegova neželjena nuspojava postala je indikacija za liječenje alopecije. U Hrvatskoj se u bezreceptnom režimu nalazi kao 2%tna i 5%tna otopina. Minoksidil koji je prisutan kao 2%tna otopina je indiciran za liječenje androgene alopecije kod muškaraca i žena u dobi od 18 do 65 godina, a 5%tna otopina je indicirana za liječenje androgene alopecije u muškaraca u dobi od 18 pa do 65 godina. (18-19) Odgovor na liječenje ovim lijekom je vrlo

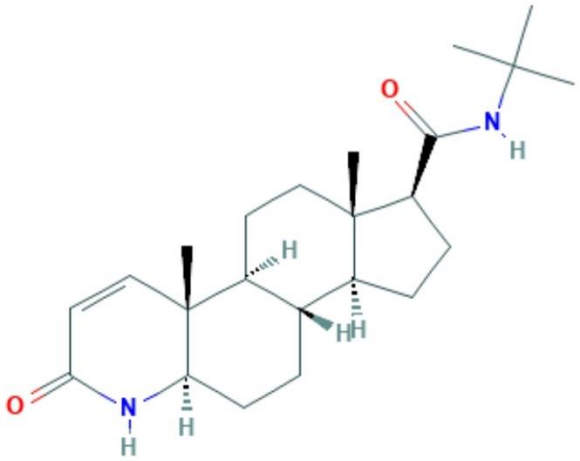
varijabilan te njegov početak djelovanja kao i stupanj ponovnog rasta kose može varirati među osobama. (18) Minoksidil je predlijek koji se prevodi u aktivni oblik minoksidil sulfat pomoću enzima sulfotransferaza. (20) Otopina minoksidila sadrži neaktivne sastojke uključujući vodu, etanol i propilenglikol koji se koriste kao nosači za povećanje topljivosti. Propilenglikol olakšava isporuku lijeka u folikul dlake, ali zbog čestih lokalnih iritacija potaknutih ovim sastojkom razvijene su formulacije otopina bez propilenglikola u obliku minoksidil pjene. Ta formulacija sadrži cetilni i stearilni alkohol te butilhidroksitoluen, a omogućuje povećanu isporuku aktivnog sastojka u ciljno mjesto uz manje iritacija u odnosu na otopinu. (21) Iako njegov mehanizam djelovanja nije u potpunosti razjašnjen zna se da skraćuje telogen i da uzrokuje rani ulazak odmarajućih folikula dlake u fazu anagena. (22) Zna se i da minoksidil otvara kalijske kanale uzrokujući hiperpolarizaciju stanične membrane i omogućujući tako više kisika i hranjivih tvari folikulima. On je i vazodilatator koji poveća protok krvi u vlasište. (3) Najčešće nuspojave otopine su svrbež i iritacija koje se povezuju s propilenglikolom u formulaciji te je u placebo kontroliranim ispitivanjima dokazana pet puta veća učestalost kod žena u odnosu na muškarce. (18) Nuspojave koje se vežu uz primjenu pjene minoksidila su glavobolja, dispneja, dermatitis, svrbež. (23) Randomizirana placebom kontrolirana studija je dokazala kako je 5% otopina u odnosu na 2% otopinu u muškaraca učinkovitija. Druga studija provedena među ženama nije dokazala superiornost 5%tne otopine nad 2%tnom, a dovela je do većih iritacija, pruritusa i hipertrihoze. (24)



Slika 6. Struktura minoksidila (25)

Finasterid je selektivni inhibitor enzima 5-alfa reduktaze koji prevodi testosteron u dihidrotestosteron (DHT). Dihidrotestosteron se veže za androgene receptore te dovodi do androgene alopecije. Dnevna doza lijeka od jednog miligrama smanjuje koncentraciju DHT

vlasišta za 64%, a razinu serumskog DHT za 68%. Javljaju se i neželjeni učinci vezani uz seksualnu disfunkciju kao što je nizak libido, erektilna disfunkcija te anorgazmija. (14)
U Hrvatskoj je registriran finasterid samo od 5 mg.

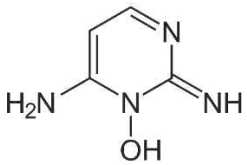


Slika 7. Struktura finasterida (26)

1.5. Aktivni sastojci

1.5.1. Aminexil

Aminexil je trgovački naziv za kopexil koji je poznat kao 2,4-diaminopirimidin-3-N-oksid. Predstavlja izmijenjeni oblik minoksidila bez nuspojava. (27) To je novi patentirani spoj koji stimulira ljudska keratinska vlakna te stoga zaustavlja gubitak kose. (28)Pomaže u smanjenju gubitka kose, a da pri tome ne mijenja strukturu kolagena te održava elastičnost tkiva koje okružuje korijen kose. (29) U preparatima dolazi kao 1.5% amineksil koji smanjuje ubrzano starenje korijena boreći se protiv procesa fibroze. (3) Često je u preparatima kombiniran s niacinamidom te piridoksinom kako bi se pojačao njegov učinak. (28) U studiji koja je provedena na štakorima Orasan i suradnici su uspoređivali učinak aminexila i minoksidila, a rezultati su pokazali značajnu superiornost u učinkovitosti minoksidila nad novim spojem. (29)



Slika 8. Struktura aminexila (28)

1.5.2. Niacinamid

Niacinamid je heterociklički aromatski spoj koji se u kozmetici koristi za njegu kože i kose. Sinonimi uključuju nikotinamid, amid nikotinske kiseline, vitamin PP, vitamin B3. (30) Dio je formulacije šampona za muškarce i žene te ampula za žene koji pomažu protiv ispadanja kose. Niacinamid je aktivni oblik vitamina B3 i komponenta koenzima nikotinamid adenin dinukleotida NAD putem kojeg je uključen u širok spektar bioloških procesa uključujući proizvodnju energije , sintezu masnih kiselina, kolesterola i steroida. (31) Radi se o netoksičnom spoju koji se brzo apsorbira kroz kožu te se široko distribuira kroz tijelo, a izlučivanje se prvenstveno vrši putem mokraćnog sustava. (30) Pojedine studije pokazuju kako je niacinamid imao učinka u poboljšanju debljine te gustoće kose dok druge navode kako se radi o vrlo slabim dokazima te studijama koje nisu bile placebom kontrolirane. U studiji su Oblong i suradnici proveli testiranje dovodi li primjena niacinamida do porasta VEGF, faktora rasta za koji se vjeruje da potiče rast kose. Testiranje je potaknuto činjenicom da se u in vitro ispitivanjima došlo do zaključka kako minoksidil povećava izvanstaničnu razinu adenozina što stimulira sintezu VEGF aktiviranjem adenozinskih receptora. Niacinamid u različitim koncentracijama nije doveo do nikakvog porasta VEGF u usporedbi s kontrolom. (32) Prema studiji provedenoj u Japanu Watanabe i suradnici su došli do zaključka kako je niacinamid doveo do blagog porasta u gustoći dlake nakon šest mjeseci korištenja losiona. Niacinamidni losion se u Japanu koristi za umjeren rast kose zbog različitih povoljnih učinaka na kožu kao što su antioksidativna te protuupalna svojstava. (33) Niacinamid se koristi desetljećima kao topikalni pripravak te je klinički ispitan u brojnim dermatološkim studijama, a do danas nije bilo naznake značajnim nuspojavama na tijelu kao ni porastu dlaka na licu. (32)

1.5.3. Piridoksin hidroklorid

Piridoksin hidroklorid je hidrokloridna sol piridoksina, vodotopljivog vitamina B6. Radi se o fotoosjetljivom spoju koji se polako razgrađuje kada je izložen svjetlu te ga iz tog razloga treba zaštititi od svjetlosti i čuvati u dobro zatvorenim spremnicima na temperaturi nižoj od 40 celzijevih stupnjeva. (34) Ovaj spoj je jedan od aktivnih sastojaka šampona protiv ispadanja kose za muškarce i žene te ampula za žene. Dolazi u kombinaciji s niacinamidom kao dodatak aminexilu kako bi se pojačao učinak aminexila na kosu. Ti dodatci imaju važnu ulogu u liječenju gubitka kose. (28) Vitamin B6 funkcionira kao stanični hranjivi sastojak koji njeguje korijen kose i pomaže u stvaranju lijepe, sjajne kose koja iznutra postaje jača te gušća. (3) Mikronutrijenti poput vitamina i minerala igraju važnu, ali ne sasvim jasnu ulogu u normalnom

razvoju folikula dlake. Ljudsko vlasište sadrži otprilike 100 000 folikula dlake, a 90% njih se nalazi u anagenoj fazi rasta te su im za rast zdrave kose neophodi vitamini, minerali i proteini. (35)

1.5.4. Arginin

Proteini su druga glavna komponenta živog organizma nakon vode. Svi proteini, uključujući one sadržane u kosi su sastavljeni od različitih aminokiselina. Za razliku od kože prisutnost i uloga prirodnih, slobodnih aminokiselina u dlačicama nisu još potpuno poznate. Zna se da aminokiseline koje se dobivaju izvana u interakciji s kosom daju različite kozmetičke učinke poput vlaženja, jačanja kose i zadržavanja umjetne boje. (36) Arginin potiče mikrocirkulaciju unoseći bitne sastojke za rast kose. (3) Oshimura i suradnici su pokazali kako arginin ima potencijalnu ulogu sidra dovodeći do taloženja druge kozmetike koja ima manji afinitet za kosu. (36) U studiji na zamorcima pokazano je kako L-arginin dovodi do povećanja duljine vanjske stanice dlake u odnosu na D-arginin te druge aminokiseline kao što je L-glutamat ili L-aspartat. (37) L-arginin je poluesencijalna aminokiselina koja sudjeluje u mnogim važnim funkcijama u ljudskom tijelu. Kao preteča dušikova oksida igra važnu ulogu u rastu kose jer upravo vazodilatacijski učinak pogoduje rastu otvarajući kalijske kanale kanale poboljšavajući opsrkbu hranjivim tvarima folikul dlake. U usporednoj studiji koja koristi proizvode za lokalnu primjenu s L-argininom pokazana je sposobnost ove aminokiseline da stimulira mikrocirkulaciju krvi te pruža esencijalne hranjive sastojke za rast. (38)

1.5.5. Kofein

Kofein je dobro poznati stimulans koji se nalazi u kavi. Sve se više istražuju njegove blagodati vezane uz rast kose s obzirom da postoji malo odobrenih lijekova za rješavanje problema alopecije. (39) Kofein je prirodni alkaloid na bazi purina koji pokazuje stimulativni učinak na rast kose zbog dobre lokalne apsorpcije. (40) On pojačava produljenje osovine dlake, produljuje anagen i potiče proliferaciju keratinocita pri čemu ženski folikul dlake pokazuje veću osjetljivost na kofein u odnosu na muški. Suprostavlja se proteinu TGF-β2 koji je odgovoran za promociju katagena te pojačava ekspresiju proteina IGF-1 kojem je uloga održavanje anagena. (39) U studiji je korištena in vivo laserska mikroskopija za ispitivanje prodiranja i skladišenja šampona koji sadrži kofein u folikul dlake. Lademann i suradnici su tom studijom pokazali kako je dovoljan kontakt od dvije minute između šampona i kose kako bi se akumulirale značajne količine šampona u folikulima dlake, a kofein je u folikulu pronađen čak

i nakon 24 sata. Nakon topikalne aplikacije kofein se može detektirati u krvi nakon 5 minuta ako je primjenjen na otvoren folikul, a nakon 15 do 20 minuta ako je primjenjen na zatvoren folikul dlake. Upravo zbog tog dokaza kako prodire do živih stanica preko folikula dlake predstavlja važan dio šampona za kosu. (41)

1.5.6. SP94 peptid

Jedan je od aktivnih sastojaka ampula protiv ispadanja kose za muškarce i žene. Peptid sp94 zahvaća korijen te se pretvara u konstruktivne elemente kose za izgradnju vlakana od korijena do vrha. (3)

1.5.7. Termalna izvorska voda

Kao dopuna ostalim sastojcima pomaže i termalna izvorska voda koja sadrži antioksidans selen. (3)

2. CILJEVI

Ciljevi ovog rada su bili:

1) Odrediti sastav preparata protiv ispadanja kose kvalitativnom analizom (GC-MS metoda)

2) Provjeriti mogući utjecaj na zdravlje

3) Usporediti deklarirane sastojke s ambalaže s identificiranim sastojcima koristeći GC-MS metodu

3. MATERIJALI I METODE

3.1.Kemikalije i uzorci za analizu

U ovom istraživanju korištene su kemikalije:

1. Kloroform, p.a., Merck, Darmstadt, Njemačka;

2. Etil acetat, p.a., Merck, Darmstadt, Njemačka;

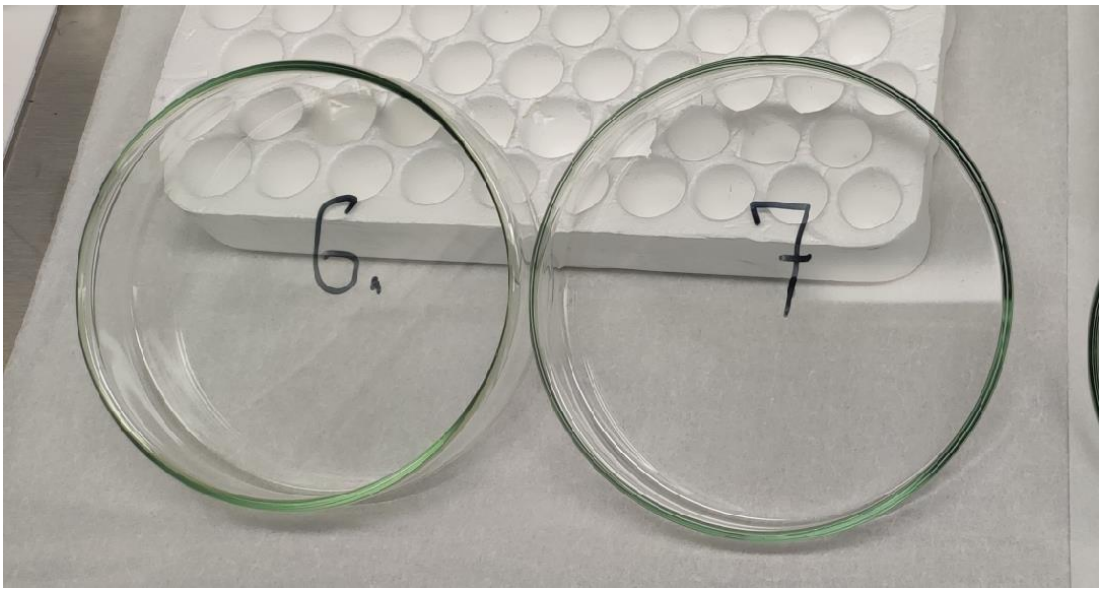
3. N-Heksan p.a., Merck, Darmstadt, Njemačka;

Provedeno je kvalitativno ispitivanje uzoraka, za određivanje njihovog sastava.

3.2.Postupak pripreme uzorka za analizu

Svi su uzorci označeni laboratorijskim brojem, a prikaz nekih od označenih uzoraka je na slici 9. Ukupno je obrađeno 3 različita pripravka za rast kose:

1. 5%tna otopina minoksidila (oznaka 6, izvješće 1)
2. Ampule za rast kose tvrtke Selective
3. Vichy ampule za žene (oznaka 7, izvješće 2)



Slika 9. Ispitivani uzorci na sušenju u digestoru

Za pripremu uzoraka korištene su staklene Petrijeve zdjelice na koje je nanesen uzorak volumena 100 µL. Uzorci su ekstrahirani smjesom organskih otapala, kloroforma, etil acetata i N-heksana u jednakom omjeru (v/v/v= 1:1:1), te su potom postavljeni u digestor na sušenje u

struji zraka. Uzorci u Petrijevim zdjelicama nekoliko su puta ispirani kloroformom kako bi se cijeli naneseni sadržaj otopio. Nakon što su otopljeni uzorci su filtrirani, preneseni su u staklene tubice za GC-MS analizu.

3.3.Instrumentalna analiza i radni uvjeti GC-MS metode

U ovom istraživanju za kvalitativnu analizu ispitivanih uzoraka korišten je plinski kromatograf s masenim spektrometrom:

Mass Hunter GC-MS Agilent Technologies

Kromatografska analiza pripremljenih ekstrakata izvedena je na plinskom kromatografu sa spektrometrom masa, metodom koja omogućava istovremeno snimanje ukupnog ionskog kromatograma (*engl. Total ion chromatogram*, TIC) u području od 40 – 600 m/z i snimanje samo odabranih iona (*engl. Single ion monitoring*, SIM). Optimiran je temperaturni program.

- Radni uvjeti:
- volumen injektiranja: 1 μL (splitless)
- temperatura injektora 250 °C
- protok plina nosioca 1,0 mL/min
- ukupno trajanje temperaturnog programa: 25 minuta:

I 100 °C izotermno 2 min

II 10 °C /min do 275 °C

III 275 °C izotermno 5 min

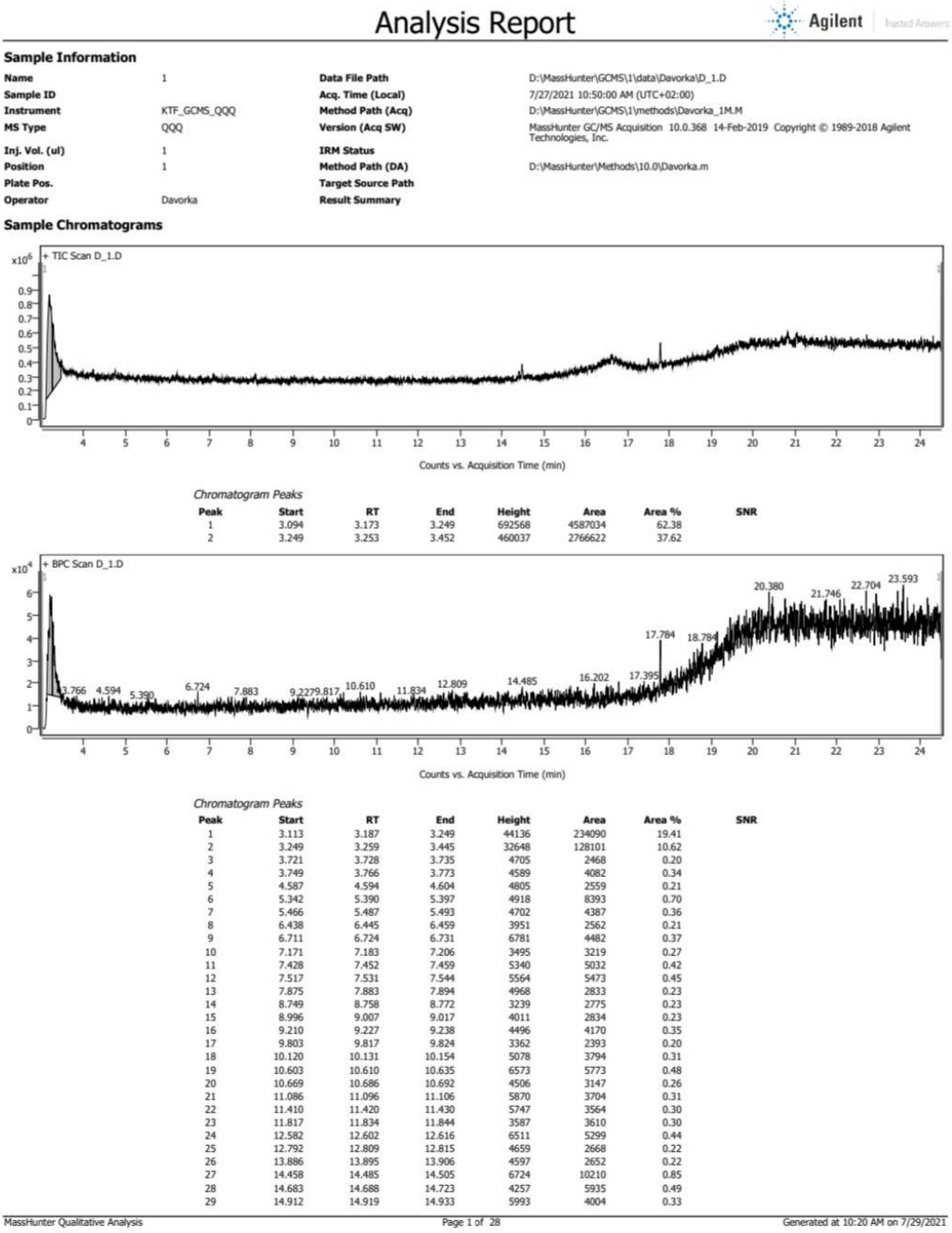
4. REZULTATI

Primijenjenom metodom pripreme uzorka te instrumentalnom tehnikom pronađeni su tragovi koji su izlistani u analitičkom izvješću. Izvješće daje dvije vrste prikaza: grafički i tablični. Grafički prikaz daje ukupni kromatogram *(Total ion chromatogram*, TIC) s popisom glavnih signala dok tablični prikaz daje detaljan popis koji uključuje podatke o vremenu izlaženja, njegovoj površini te udjelu u svim pronađenim signalima. U tabličnom prikazu su dati podatci usporedbe s bazama podataka s mogućim upućivanjem o eventualnoj pronađenoj tvari. Usporedba se bazira na primjeni komercijalnih biblioteka spojeva i postotkom podudaranja.

U grafičkom prikazu x os prikazuje vrijeme izlaženja, a y os predstavlja intenzitet signala koji je proporcionalan količini pronađene tvari. U ovom istraživanju radila se isključivo kvalitativna analiza.

Među pomoćnim tvarima u otopini minoksidila za kožu vlasišta koja je registrirana kao lijek za poticanje rasta kose navedeni su pročišćena voda, propilenglikol te etanol (96%). (19) Kvalitativnom analizom su pronađene još brojne tvari koje se ne nalaze na popisu međutim prema visini signala možemo zaključiti da se nalaze u tragovima ili predstavljaju šum instrumenta što se ne smatra signalom pronađene tvari.

Primjer rezultata dobivenih analizom uzorka br. 1 koristeći GC-MS metodu, prikazani su grafički i tablično.



Analysis Report

Agilent

Sample Information

Name	1	**Data File Path**	D:\MassHunter\GCMS\1\data\Davorka\D_1.D
Sample ID		**Acq. Time (Local)**	7/27/2021 10:50:00 AM (UTC+02:00)
Instrument	KTF_GCMS_QQQ	**Method Path (Acq)**	D:\MassHunter\GCMS\1\methods\Davorka_1M.M
MS Type	QQQ	**Version (Acq SW)**	MassHunter GC/MS Acquisition 10.0.368 14-Feb-2019 Copyright © 1989-2018 Agilent Technologies, Inc.
Inj. Vol. (ul)	1	**IRM Status**	
Position	1	**Method Path (DA)**	D:\MassHunter\Methods\10.0\Davorka.m
Plate Pos.		**Target Source Path**	
Operator	Davorka	**Result Summary**	

Sample Chromatograms

Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area %	SNR
1	3.094	3.173	3.249	692568	4587034	62.38	
2	3.249	3.253	3.452	460037	2766622	37.62	

Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area %	SNR
1	3.113	3.187	3.249	44136	234090	19.41	
2	3.249	3.259	3.445	32648	128101	10.62	
3	3.721	3.728	3.735	4705	2468	0.20	
4	3.749	3.766	3.773	4589	4082	0.34	
5	4.587	4.594	4.604	4805	2559	0.21	
6	5.342	5.390	5.397	4918	8393	0.70	
7	5.466	5.487	5.493	4702	4387	0.36	
8	6.438	6.445	6.459	3951	2562	0.21	
9	6.711	6.724	6.731	6781	4482	0.37	
10	7.171	7.183	7.206	3495	3219	0.27	
11	7.428	7.452	7.459	5340	5032	0.42	
12	7.517	7.531	7.544	5564	5473	0.45	
13	7.875	7.883	7.894	4968	2833	0.23	
14	8.749	8.758	8.772	3239	2775	0.23	
15	8.996	9.007	9.017	4011	2834	0.23	
16	9.210	9.227	9.238	4496	4170	0.35	
17	9.803	9.817	9.824	3362	2393	0.20	
18	10.120	10.131	10.154	5078	3794	0.31	
19	10.603	10.610	10.635	6573	5773	0.48	
20	10.669	10.686	10.692	4506	3147	0.26	
21	11.086	11.096	11.106	5870	3704	0.31	
22	11.410	11.420	11.430	5747	3564	0.30	
23	11.817	11.834	11.844	3587	3610	0.30	
24	12.582	12.602	12.616	6511	5299	0.44	
25	12.792	12.809	12.815	4659	2668	0.22	
26	13.886	13.895	13.906	4597	2652	0.22	
27	14.458	14.485	14.505	6724	10210	0.85	
28	14.683	14.688	14.723	4257	5935	0.49	
29	14.912	14.919	14.933	5993	4004	0.33	

Slika 10.

Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area %	SNR
30	15.599	15.605	15.614	5446	2660	0.22	
31	15.633	15.640	15.650	6819	3448	0.29	
32	15.965	15.991	15.997	3982	3882	0.32	
33	16.026	16.036	16.047	3730	2888	0.24	
34	16.175	16.181	16.191	5975	2929	0.24	
35	16.192	16.202	16.208	7990	3365	0.28	
36	16.262	16.271	16.295	4239	3973	0.33	
37	16.402	16.409	16.433	3841	4946	0.41	
38	16.440	16.498	16.525	7885	18582	1.54	
39	16.531	16.536	16.545	5621	2620	0.22	
40	16.591	16.602	16.612	7167	5001	0.41	
41	16.778	16.788	16.798	8451	4128	0.34	
42	17.291	17.305	17.312	5939	3611	0.30	
43	17.385	17.395	17.403	5622	3112	0.26	
44	17.768	17.784	17.801	21949	18792	1.56	
45	17.901	17.915	17.929	6229	6003	0.50	
46	18.020	18.026	18.046	6150	4848	0.40	
47	18.175	18.181	18.210	7189	5981	0.50	
48	18.405	18.412	18.419	8617	4194	0.35	
49	18.447	18.481	18.489	7923	7272	0.60	
50	18.502	18.505	18.521	5481	3138	0.26	
51	18.658	18.667	18.693	10127	9729	0.81	
52	18.699	18.712	18.724	6917	6131	0.51	
53	18.732	18.743	18.753	12309	8165	0.68	
54	18.760	18.784	18.817	15075	21514	1.78	
55	19.136	19.143	19.160	10685	7685	0.64	
56	19.444	19.453	19.461	10765	6139	0.51	
57	19.482	19.508	19.522	10830	14292	1.18	
58	19.550	19.556	19.574	6326	4868	0.40	
59	19.605	19.615	19.622	7638	2766	0.23	
60	19.784	19.791	19.801	8722	4436	0.37	
61	19.833	19.839	19.856	11168	6248	0.52	
62	19.999	20.039	20.073	9801	21107	1.75	
63	20.095	20.111	20.120	9517	6003	0.50	
64	20.127	20.142	20.164	10600	13581	1.13	
65	20.194	20.204	20.218	11789	10001	0.83	
66	20.329	20.380	20.387	15915	18192	1.51	
67	20.456	20.466	20.473	13859	7159	0.59	
68	20.546	20.573	20.587	7516	13328	1.11	
69	20.632	20.656	20.669	7301	10431	0.86	
70	20.691	20.725	20.742	7903	12991	1.08	
71	20.756	20.763	20.770	12937	5246	0.43	
72	20.784	20.787	20.801	9582	5190	0.43	
73	20.846	20.849	20.859	8275	5150	0.43	
74	20.874	20.891	20.908	9741	11283	0.94	
75	20.915	20.922	20.932	9191	4718	0.39	
76	20.973	20.984	20.995	10742	7878	0.65	
77	21.050	21.073	21.082	7575	8921	0.74	
78	21.111	21.125	21.142	10863	12382	1.03	
79	21.146	21.159	21.171	12017	10633	0.88	
80	21.179	21.184	21.194	8778	3692	0.31	
81	21.230	21.239	21.245	10530	5092	0.42	
82	21.387	21.394	21.404	9683	5283	0.44	
83	21.432	21.439	21.469	7853	9546	0.79	
84	21.546	21.552	21.563	10000	6019	0.50	
85	21.625	21.635	21.642	8953	5519	0.46	
86	21.663	21.687	21.697	8193	12314	1.02	
87	21.707	21.718	21.735	11354	7945	0.66	
88	21.739	21.746	21.759	12018	7696	0.64	
89	21.814	21.828	21.835	9212	5950	0.49	
90	21.839	21.856	21.862	9092	7759	0.64	
91	21.880	21.883	21.894	8558	3551	0.29	
92	21.939	21.945	21.960	9544	6157	0.51	
93	21.978	22.001	22.011	7237	8340	0.69	
94	22.073	22.080	22.091	11644	5195	0.43	
95	22.171	22.176	22.187	12276	5503	0.46	
96	22.187	22.201	22.210	8979	6269	0.52	
97	22.346	22.356	22.374	9684	9874	0.82	
98	22.380	22.397	22.404	9897	7691	0.64	
99	22.580	22.594	22.599	10127	5187	0.43	
100	22.627	22.638	22.645	8030	5313	0.44	
101	22.694	22.704	22.725	17055	12523	1.04	
102	22.769	22.787	22.793	9382	7265	0.60	
103	22.845	22.880	22.893	11109	14629	1.21	
104	22.931	22.942	22.969	15896	16265	1.35	
105	22.973	22.983	22.990	9968	4814	0.40	
106	22.998	23.007	23.018	10891	6856	0.57	
107	23.080	23.087	23.097	6386	3971	0.33	
108	23.109	23.114	23.132	10455	6927	0.57	
109	23.143	23.169	23.177	10206	12235	1.01	
110	23.222	23.228	23.262	8557	12305	1.02	
111	23.283	23.293	23.323	9843	13979	1.16	
112	23.338	23.345	23.358	10875	7437	0.62	
113	23.407	23.414	23.421	10322	5799	0.48	
114	23.449	23.459	23.466	16995	8685	0.72	
115	23.552	23.559	23.566	12248	6876	0.57	
116	23.576	23.593	23.607	20308	19742	1.64	

Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area %	SNR
117	23.835	23.842	23.852	14438	8807	0.73	
118	24.005	24.011	24.017	7757	3031	0.25	
119	24.166	24.169	24.180	12076	4318	0.36	
120	24.228	24.242	24.252	7412	5428	0.45	
121	24.259	24.269	24.286	7944	6921	0.57	
122	24.467	24.483	24.495	12328	11688	0.97	

Sample Spectra

+ Scan (rt: 3.10-3.25 min) **Peak 1 from + TIC Scan (Oxirane; C2H4O)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Oxirane	C2H4O				75-21-8	59.32	59.32			W9N08.L
No	LibSearch	Rimantadine	C12H21N				13392-28-4	58.17	58.17			W9N08.L
No	LibSearch	N-Chlorodimethylamine	C2H6ClN				1585-74-6	57.86	57.86			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Oxirane	C2H4O		75-21-8			59.32	59.32			W9N08.L

+ Scan (rt: 3.25-3.45 min) **Peak 2 from + TIC Scan ((1S,2S,4S)-N-Benzyl-2-methylsulfonylamino-7,7-dimethylbicyclo[2.2.1]hept-1-y...; C18H28N2O4S2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(1S,2S,4S)-N-Benzyl-2-methylsulfonylamino-7,7-dimethylbicyclo[2.2.1]hept-1-y...	C18H28N2O4S2				999659-60-5	61.34	61.34			W9N08.L
No	LibSearch	N-((15)N-NITRO)-DIMETHYLAMINE	C2H6N2O2				53798-88-2	60.74	60.74			W9N08.L
No	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-	C9H13NO				48115-38-4	58.58	58.58			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(1S,2S,4S)-N-Benzyl-2-methylsulfonylamino-7,7-dimethylbicyclo[2.2.1]hept-1-y...	C18H28N2O4S2		999659-60-5			61.34	61.34			W9N08.L

+ Scan (rt: 3.12-3.25 min) **Peak 1 from + BPC Scan (Carbamic acid, methyl ester; C2H5NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Carbamic acid, methyl ester	C2H5NO2				598-55-0	64.99	64.99			W9N08.L
No	LibSearch	Oxirane	C2H4O				75-21-8	64.66	64.66			W9N08.L
No	LibSearch	Acetaldehyde	C2H4O				75-07-0	60.33	60.33			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Carbamic acid, methyl ester	C2H5NO2		598-55-0			64.99	64.99			W9N08.L

+ Scan (rt: 3.25-3.44 min) **Peak 2 from + BPC Scan ((1S,2S,4S)-N-Benzyl-2-methylsulfonylamino-7,7-dimethylbicyclo[2.2.1]hept-1-y...; C18H28N2O4S2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(1S,2S,4S)-N-Benzyl-2-methylsulfonylamino-7,7-dimethylbicyclo[2.2.1]hept-1-y...	C18H28N2O4S2				999659-60-5	61.34	61.34			W9N08.L
No	LibSearch	N-((15)N-NITRO)-DIMETHYLAMINE	C2H6N2O2				53798-88-2	60.83	60.83			W9N08.L
No	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-	C9H13NO				48115-38-4	58.69	58.69			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(1S,2S,4S)-N-Benzyl-2-methylsulfonylamino-7,7-dimethylbicyclo[2.2.1]hept-1-y...	C18H28N2O4S2		999659-60-5			61.34	61.34			W9N08.L

+ Scan (rt: 3.72-3.73 min) **Peak 3 from + BPC Scan (N-chloro-N,N-dimethylamine ; C2H6ClN)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	N-chloro-N,N-dimethylamine	C2H6ClN				1585-74-6	53.71	53.71			W9N08.L
No	LibSearch	N-Chlorodimethylamine	C2H6ClN				1585-74-6	53.09	53.09			W9N08.L
No	LibSearch	N-chloro-N,N-dimethylamine	C2H6ClN				1585-74-6	53.05	53.05			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	N-chloro-N,N-dimethylamine	C2H6ClN		1585-74-6			53.71	53.71			W9N08.L

+ Scan (rt: 3.75-3.77 min) **Peak 4 from + BPC Scan (Carbamic acid, methyl ester; C2H5NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Carbamic acid, methyl ester	C2H5NO2				598-55-0	57.58	57.58			W9N08.L
No	LibSearch	Oxirane	C2H4O				75-21-8	50.65	50.65			W9N08.L
No	LibSearch	Acetaldehyde	C2H4O				75-07-0	50.61	50.61			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Carbamic acid, methyl ester	C2H5NO2		598-55-0			57.58	57.58			W9N08.L

+ Scan (rt: 4.59-4.60 min) **Peak 5 from + BPC Scan (Carbamic acid, methyl ester; C2H5NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Carbamic acid, methyl ester	C2H5NO2				598-55-0	59.61	59.61			W9N08.L
No	LibSearch	Acetamide, 2-fluoro-	C2H4FNO				640-19-7	56.20	56.20			W9N08.L
No	LibSearch	Acetamide, 2-fluoro-	C2H4FNO				640-19-7	54.19	54.19			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Carbamic acid, methyl ester	C2H5NO2		598-55-0			59.61	59.61			W9N08.L

+ Scan (rt: 5.35-5.39 min) **Peak 6 from + BPC Scan**

+ Scan (rt: 5.47-5.49 min) **Peak 7 from + BPC Scan (Cathinone ; C9H11NO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Cathinone	C9H11NO				71031-15-7	52.25	52.25			W9N08.L
No	LibSearch	Ethinamate	C9H13NO2				126-52-3	51.97	51.97			W9N08.L
No	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-, [R-(R*,S*)]-	C9H13NO				492-41-1	51.90	51.90			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Cathinone	C9H11NO		71031-15-7			52.25	52.25			W9N08.L

+ Scan (rt: 6.44-6.46 min) **Peak 8 from + BPC Scan (Ethanol, 2-(methylamino)- ; C3H9NO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Ethanol, 2-(methylamino)-	C3H9NO				109-83-1	52.01	52.01			W9N08.L
No	LibSearch	Ethanol, 2-(methylamino)-	C3H9NO				109-83-1	51.54	51.54			W9N08.L
No	LibSearch	Ethanol, 2-(methylamino)-	C3H9NO				109-83-1	51.17	51.17			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Ethanol, 2-(methylamino)-	C3H9NO		109-83-1			52.01	52.01			W9N08.L

+ Scan (rt: 6.71-6.73 min) **Peak 9 from + BPC Scan (Ethane, 2-chloro-1,1-dimethoxy- ; C4H9ClO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Ethane, 2-chloro-1,1-dimethoxy-	C4H9ClO2				97-97-2	53.09	53.09			W9N08.L
No	LibSearch	Ethane, 2-chloro-1,1-dimethoxy-	C4H9ClO2				97-97-2	53.05	53.05			W9N08.L
No	LibSearch	Ethane, 2-chloro-1,1-dimethoxy-	C4H9ClO2				97-97-2	51.76	51.76			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Ethane, 2-chloro-1,1-dimethoxy-	C4H9ClO2		97-97-2			53.09	53.09			W9N08.L

+ Scan (rt: 7.17-7.20 min) **Peak 10 from + BPC Scan**

+ Scan (rt: 7.43-7.46 min) **Peak 11 from + BPC Scan (N-Benzenesulfonylazetidin-3-one ; C9H9NO3S)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	N-Benzenesulfonylazetidin-3-one	C9H9NO3S				82380-59-4	53.65	53.65			W9N08.L
No	LibSearch	N-Benzenesulfonylazetidin-3-one	C9H9NO3S				82380-59-4	53.28	53.28			W9N08.L
No	LibSearch	[4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene] (name from MOL file)	C15H24				999192-33-4	51.10	51.10			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	N-Benzenesulfonylazetidin-3-one	C9H9NO3S		82380-59-4			53.65	53.65			W9N08.L

+ Scan (rt: 7.52-7.54 min) **Peak 12 from + BPC Scan (Carbamic acid, methyl ester; C2H5NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Carbamic acid, methyl ester	C2H5NO2				598-55-0	65.30	65.30			W9N08.L
No	LibSearch	Acetaldehyde	C2H4O				75-07-0	57.57	57.57			W9N08.L
No	LibSearch	Oxirane	C2H4O				75-21-8	57.07	57.07			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Carbamic acid, methyl ester	C2H5NO2		598-55-0			65.30	65.30			W9N08.L

+ Scan (rt: 7.88-7.89 min) **Peak 13 from + BPC Scan (Benzenemethanol, .alpha.-(1-aminoethyl)-; C9H13NO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-	C9H13NO				48115-38-4	62.57	62.57			W9N08.L
No	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-, [R-(R*,S*)]-	C9H13NO				492-41-1	59.53	59.53			W9N08.L
No	LibSearch	Cathine	C9H13NO				492-39-7	57.50	57.50			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Benzenemethanol, .alpha.-(1-aminoethyl)-	C9H13NO		48115-38-4			62.57	62.57			W9N08.L

+ Scan (rt: 8.75-8.77 min) **Peak 14 from + BPC Scan (N-Chlorodimethylamine ; C2H6ClN)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	N-Chlorodimethylamine	C2H6ClN				1585-74-6	59.85	59.85			W9N08.L
No	LibSearch	N-chloro-N,N-dimethylamine	C2H6ClN				1585-74-6	59.38	59.38			W9N08.L
No	LibSearch	N-Chlorodimethylamine	C2H6ClN				1585-74-6	58.73	58.73			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	N-Chlorodimethylamine	C2H6ClN		1585-74-6			59.85	59.85			W9N08.L

+ Scan (rt: 9.00-9.01 min) **Peak 15 from + BPC Scan ((Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...; C19H28O7S2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...	C19H28O7S2				999698-32-9	57.24	57.24			W9N08.L
No	LibSearch	(E)-Methyl 2-{1'-[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl]-2'-[...	C27H38O7S2Si				999769-68-0	55.61	55.61			W9N08.L
No	LibSearch	(E)-Methyl 2-{[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl](formyl...	C23H36O6S2Si				0-00-0	54.95	54.95			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...	C19H28O7S2		999698-32-9			57.24	57.24			W9N08.L

+ Scan (rt: 9.21-9.23 min) **Peak 16 from + BPC Scan (N-Benzyl-N'-[(2,2-dimethoxy)-1-phenylethyl]-(2R,3R)-2,3-di-O-isopropylidenet...; C25H31NO7)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	N-Benzyl-N'-[(2,2-dimethoxy)-1-phenylethyl]-(2R,3R)-2,3-di-O-isopropylidenet...	C25H31NO7				999720-53-2	51.89	51.89			W9N08.L
No	LibSearch	benzyl 4.beta.-dimethoxymethyl-2.alpha.,3.alpha.-(isopropylidendioxy)cyclope...	C19H26O6				104748-74-5	51.65	51.65			W9N08.L
No	LibSearch	2-(Benzyloxy)-4-(hydroxymethyl)oct-6-enal - Dimethyl Acetal	C18H30O4				0-00-0	50.13	50.13			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	N-Benzyl-N'-[(2,2-dimethoxy)-1-phenylethyl]-(2R,3R)-2,3-di-O-isopropylidenet...	C25H31NO7		999720-53-2			51.89	51.89			W9N08.L

+ Scan (rt: 9.81-9.82 min) **Peak 17 from + BPC Scan**

+ Scan (rt: 10.12-10.15 min) **Peak 18 from + BPC Scan (Rimantadine ; C12H21N)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Rimantadine	C12H21N				13392-28-4	53.51	53.51			W9N08.L
No	LibSearch	(1S,2S,4S)-N-Benzyl-2-methylsulfonylamino-7,7-dimethylbicyclo[2.2.1]hept-1-y...	C18H28N2O4S2				999659-60-5	51.56	51.56			W9N08.L
No	LibSearch	1.alpha.,8.alpha.-Dimethyl-1,4,4a.beta.,4b.beta.,5,8,8a.beta.,9a.alpha.-octa...	C15H20O				999224-42-6	50.85	50.85			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Rimantadine	C12H21N		13392-28-4			53.51	53.51			W9N08.L

+ Scan (rt: 10.61-10.63 min) **Peak 19 from + BPC Scan (Ethanol, 2-(methylamino)- ; C3H9NO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Ethanol, 2-(methylamino)-	C3H9NO				109-83-1	52.97	52.97			W9N08.L
No	LibSearch	Ethanol, 2-(methylamino)-	C3H9NO				109-83-1	52.93	52.93			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Ethanol, 2-(methylamino)-	C3H9NO		109-83-1			52.97	52.97			W9N08.L

+ Scan (rt: 10.67-10.69 min) **Peak 20 from + BPC Scan (Acetamide, 2-fluoro- ; C2H4FNO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Acetamide, 2-fluoro-	C2H4FNO				640-19-7	59.09	59.09			W9N08.L
No	LibSearch	Acetamide, 2-fluoro-	C2H4FNO				640-19-7	58.60	58.60			W9N08.L
No	LibSearch	1,1,1,2,3,3-Hexafluoro-4-methylpentane	C6H8F6				53072-71-2	56.37	56.37			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Acetamide, 2-fluoro-	C2H4FNO		640-19-7			59.09	59.09			W9N08.L

+ Scan (rt: 11.09-11.10 min) **Peak 21 from + BPC Scan (Carbamic acid, methyl ester; C2H5NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Carbamic acid, methyl ester	C2H5NO2				598-55-0	59.85	59.85			W9N08.L
No	LibSearch	(2E,4E)-N-Isopropyl-7-phenyl-6-oxo-2,4-heptadienamide	C16H19NO2				999340-03-0	57.41	57.41			W9N08.L
No	LibSearch	5-Amino-2-methylhexan-2-ol	C7H17NO				999038-00-8	53.40	53.40			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Carbamic acid, methyl ester	C2H5NO2		598-55-0			59.85	59.85			W9N08.L

+ Scan (rt: 11.41-11.43 min) **Peak 22 from + BPC Scan (Pyridinium N-(5'-Bromo-3'-fluoropyridin-2'-yl)aminide; C10H7BrFN3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Pyridinium N-(5'-Bromo-3'-fluoropyridin-2'-yl)aminide	C10H7BrFN3				0-00-0	55.49	55.49			W9N08.L
No	LibSearch	1-BROMO-2-AMINOPROPANE	C3H8BrN				72696-68-5	52.84	52.84			W9N08.L
No	LibSearch	N-Chlorodimethylamine	C2H6ClN				1585-74-6	51.05	51.05			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Pyridinium N-(5'-Bromo-3'-fluoropyridin-2'-yl)aminide	C10H7BrFN3		0-00-0			55.49	55.49			W9N08.L

+ Scan (rt: 11.82-11.84 min) **Peak 23 from + BPC Scan (Benzenemethanol, .alpha.-(1-aminoethyl)-; C9H13NO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-	C9H13NO				48115-38-4	54.38	54.38			W9N08.L
No	LibSearch	Rimantadine	C12H21N				13392-28-4	53.75	53.75			W9N08.L
No	LibSearch	1,2-Bis(3,4-dibromocyclohexyl)-1,2-dibromoethane	C14H20Br6				999784-74-5	52.70	52.70			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Benzenemethanol, .alpha.-(1-aminoethyl)-	C9H13NO		48115-38-4			54.38	54.38			W9N08.L

+ Scan (rt: 12.59-12.61 min) **Peak 24 from + BPC Scan (Benzenemethanol, .alpha.-(1-aminoethyl)-, [R-(R*,S*)]-; C9H13NO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-, [R-(R*,S*)]-	C9H13NO				492-41-1	60.98	60.98			W9N08.L
No	LibSearch	Acetamide, 2-fluoro-	C2H4FNO				640-19-7	55.38	55.38			W9N08.L
No	LibSearch	Benzenemethanol, .alpha.-(1-aminoethyl)-	C9H13NO				48115-38-4	54.56	54.56			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Benzenemethanol, .alpha.-(1-aminoethyl)-, [R-(R*,S*)]-	C9H13NO		492-41-1			60.98	60.98			W9N08.L

+ Scan (rt: 12.80-12.81 min) **Peak 25 from + BPC Scan (Carbamic acid, methyl ester; C2H5NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Carbamic acid, methyl ester	C2H5NO2				598-55-0	76.58	76.58			W9N08.L
No	LibSearch	Ethanol, 2-(methylamino)-	C3H9NO				109-83-1	69.67	69.67			W9N08.L
No	LibSearch	Oxirane	C2H4O				75-21-8	69.66	69.66			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Carbamic acid, methyl ester	C2H5NO2		598-55-0			76.58	76.58			W9N08.L

+ Scan (rt: 13.89-13.90 min) **Peak 26 from + BPC Scan ((E)-Methyl 2-{1'-[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl]-2'-[...; C27H38O7S2Si)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(E)-Methyl 2-{1'-[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl]-2'-[...	C27H38O7S2Si				999769-68-0	64.29	64.29			W9N08.L
No	LibSearch	Methyl 2-(2'-tert-Butydimethylsilyloxy-1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"...	C21H40O6S2Si				999736-31-8	59.45	59.45			W9N08.L
No	LibSearch	Methyl 2-([2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]formylmethoxymeth..	C15H24O6S2				999601-38-9	59.01	59.01			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(E)-Methyl 2-{1'-[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl]-2'-[...	C27H38O7S2Si		999769-68-0			64.29	64.29			W9N08.L

+ Scan (rt: 14.46-14.50 min) **Peak 27 from + BPC Scan (5-(1-Dimethylaminoethylidene)cyclopenta-1,3-dienyl]hydroxyacetic acid ethyl ...; C13H19NO3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	5-(1-Dimethylaminoethylidene)cyclopenta-1,3-dienyl]hydroxyacetic acid ethyl ...	C13H19NO3				999283-03-6	69.23	69.23			W9N08.L
No	LibSearch	1-(dodecycloxy)-4-methoxybutan-2-one	C17H34O3				114250-56-5	62.13	62.13			W9N08.L
No	LibSearch	1-D1-1,2,4-TRIAZOLE	C2H2DN3				39787-01-4	55.73	55.73			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	5-(1-Dimethylaminoethylidene)cyclopenta-1,3-dienyl]hydroxyacetic acid ethyl ...	C13H19NO3		999283-03-6			69.23	69.23			W9N08.L

+ Scan (rt: 14.68-14.72 min) **Peak 28 from + BPC Scan (3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole; C15H17N3OS)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	63.35	63.35			W9N08.L
No	LibSearch	benzyl 2,2'-di-O-methylstenosporate	C32H38O7				0-00-0	60.49	60.49			W9N08.L
No	LibSearch	benzyl 2,2'-di-O-methyldivaricatate	C30H34O7				999750-48-5	60.47	60.47			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS		999422-75-2			63.35	63.35			W9N08.L

+ Scan (rt: 14.92-14.93 min) **Peak 29 from + BPC Scan**

+ Scan (rt: 15.60-15.61 min) **Peak 30 from + BPC Scan ((Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...; C19H28O7S2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...	C19H28O7S2				999698-32-9	65.96	65.96			W9N08.L
No	LibSearch	(E)-Methyl 2-{[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl](formyl...	C23H36O6S2Si				0-00-0	62.43	62.43			W9N08.L
No	LibSearch	3-[o-Methoxyphenyl]-5,6-{(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	60.39	60.39			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...	C19H28O7S2		999698-32-9			65.96	65.96			W9N08.L

+ Scan (rt: 15.64-15.65 min) **Peak 31 from + BPC Scan ((Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...; C19H28O7S2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...	C19H28O7S2				999698-32-9	58.67	58.67			W9N08.L
No	LibSearch	(E)-Methyl 2-{1'-[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl]-2'-[...	C27H38O7S2Si				999769-68-0	56.50	56.50			W9N08.L
No	LibSearch	(E)-Methyl 2-{[2"-(2"',2"'-dimethoxyethyl)-1",3"-dithiane-2"-yl](formyl...	C23H36O6S2Si				0-00-0	56.13	56.13			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(Z)-Methyl 2-{1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2""-...	C19H28O7S2		999698-32-9			58.67	58.67			W9N08.L

+ Scan (rt: 15.97-15.99 min) **Peak 32 from + BPC Scan (1-Phenyl-3-((trimethylsilyl)oxy)-5-hepten-4-one; C16H24O2Si)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1-Phenyl-3-((trimethylsilyl)oxy)-5-hepten-4-one	C16H24O2Si				72252-12-1	53.77	53.77			W9N08.L
No	LibSearch	2,3-Dimethyl-1-[1',2',3'-tris(t-butyl)cyclopropenyl]-2-buten-1-one	C21H36O				999469-65-3	52.84	52.84			W9N08.L
No	LibSearch	Benzenepropanoic acid, tert-butyldimethylsilyl ester	C15H24O2Si				78324-01-3	52.72	52.72			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1-Phenyl-3-((trimethylsilyl)oxy)-5-hepten-4-one	C16H24O2Si		72252-12-1			53.77	53.77			W9N08.L

+ Scan (rt: 16.03-16.04 min) **Peak 33 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	52.10	52.10			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			52.10	52.10			W9N08.L

+ Scan (rt: 16.18-16.19 min) **Peak 34 from + BPC Scan (N-(tert-Butoxycarbonyl)-2-methyl-4,4-diphenylbut-3-enamine; C22H27NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	N-(tert-Butoxycarbonyl)-2-methyl-4,4-diphenylbut-3-enamine	C22H27NO2				999548-21-3	59.93	59.93			W9N08.L
No	LibSearch	1,2-bis[1,2,3-tri(t-Butyl)-2-cyclopropen-1-yl] 1,2-ethanedione	C32H54O2				105562-63-8	58.28	58.28			W9N08.L
No	LibSearch	1,2,3-tri (t-Butyl)cyclopropenylium-hydrogene dichloride	C15H28Cl2				105562-65-0	58.28	58.28			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	N-(tert-Butoxycarbonyl)-2-methyl-4,4-diphenylbut-3-enamine	C22H27NO2		999548-21-3			59.93	59.93			W9N08.L

+ Scan (rt: 16.19-16.21 min) **Peak 35 from + BPC Scan (1,2,3-tri(t-Butyl)cyclopropenylium tribromide; C15H27Br3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1,2,3-tri(t-Butyl)cyclopropenylium tribromide	C15H27Br3				142634-81-9	60.09	60.09			W9N08.L
No	LibSearch	Nonahexacontanoic acid, methyl ester	C70H140O2				40710-36-9	59.82	59.82			W9N08.L
No	LibSearch	Octacosane	C28H58				630-02-4	56.70	56.70			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1,2,3-tri(t-Butyl)cyclopropenylium tribromide	C15H27Br3		142634-81-9			60.09	60.09			W9N08.L

+ Scan (rt: 16.26-16.29 min) **Peak 36 from + BPC Scan (1,2,3-tri (t-Butyl)cyclopropenylium-hydrogene dichloride; C15H28Cl2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1,2,3-tri (t-Butyl)cyclopropenylium-hydrogene dichloride	C15H28Cl2				105562-65-0	56.04	56.04			W9N08.L
No	LibSearch	1,4-Dihydro-3,6-bis[1,2,3-tri(t-butyl)-2-cyclopropen-1-yl] 1,2,4,5-tetrazine	C32H56N4				142634-77-3	56.04	56.04			W9N08.L
No	LibSearch	1,2-bis[1,2,3-tri(t-Butyl)-2-cyclopropen-1-yl] 1,2-ethanedione	C32H54O2				105562-63-8	56.04	56.04			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1,2,3-tri (t-Butyl)cyclopropenylium-hydrogene dichloride	C15H28Cl2		105562-65-0			56.04	56.04			W9N08.L

+ Scan (rt: 16.41-16.43 min) **Peak 37 from + BPC Scan (N-[(dimethylamino)(t-butylthio)methylene]-benzamide; C14H20N2OS)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	N-[(dimethylamino)(t-butylthio)methylene]-benzamide	C14H20N2OS				999358-48-6	55.43	55.43			W9N08.L
No	LibSearch	2,3-Dimethyl-1-[1',2',3'-tris(t-butyl)cyclopropenyl]-2-buten-1-one	C21H36O				999469-65-3	52.56	52.56			W9N08.L
No	LibSearch	1,2,3-tri(t-Butyl)cyclopropenylium trichloride	C15H27Cl3				142634-80-8	50.86	50.86			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	N-[(dimethylamino)(t-butylthio)methylene]-benzamide	C14H20N2OS		999358-48-6			55.43	55.43			W9N08.L

+ Scan (rt: 16.44-16.52 min) **Peak 38 from + BPC Scan (2,3-Dimethyl-1-[1',2',3'-tris(t-butyl)cyclopropenyl]-2-buten-1-one; C21H36O)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	2,3-Dimethyl-1-[1',2',3'-tris(t-butyl)cyclopropenyl]-2-buten-1-one	C21H36O				999469-65-3	63.29	63.29			W9N08.L
No	LibSearch	Nonacosane	C29H60				630-03-5	59.13	59.13			W9N08.L
No	LibSearch	Octacosane	C28H58				630-02-4	58.86	58.86			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	2,3-Dimethyl-1-[1',2',3'-tris(t-butyl)cyclopropenyl]-2-buten-1-one	C21H36O		999469-65-3			63.29	63.29			W9N08.L

+ Scan (rt: 16.53-16.54 min) **Peak 39 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	59.75	59.75			W9N08.L
No	LibSearch	2-[1',2',3'-tris(t-Butyl)]cyclopropenyl-2-diazo-3,3-dimethylbutan-2-one	C21H36N2O				0-00-0	55.72	55.72			W9N08.L
No	LibSearch	1,2,3-tri(t-Butyl)cyclopropenylium trichloride	C15H27Cl3				142634-80-8	55.37	55.37			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			59.75	59.75			W9N08.L

+ Scan (rt: 16.59-16.61 min) **Peak 40 from + BPC Scan (1,2,3-tri(t-Butyl)cyclopropenylium trichloride; C15H27Cl3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1,2,3-tri(t-Butyl)cyclopropenylium trichloride	C15H27Cl3				142634-80-8	56.51	56.51			W9N08.L
No	LibSearch	2-[1',2',3'-tris(t-Butyl)]cyclopropenyl-2-diazo-3,3-dimethylbutan-2-one	C21H36N2O				0-00-0	56.25	56.25			W9N08.L
No	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	54.85	54.85			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1,2,3-tri(t-Butyl)cyclopropenylium trichloride	C15H27Cl3		142634-80-8			56.51	56.51			W9N08.L

+ Scan (rt: 16.78-16.79 min) **Peak 41 from + BPC Scan (3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole; C15H17N3OS)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	53.71	53.71			W9N08.L
No	LibSearch	benzyl 4'-O-benzylsubmerochloropheiate	C36H38O8				0-00-0	52.74	52.74			W9N08.L
No	LibSearch	benzyl 2,2'-di-O-methyldivaricatate	C30H34O7				999750-48-5	52.74	52.74			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS		999422-75-2			53.71	53.71			W9N08.L

+ Scan (rt: 17.29-17.31 min) **Peak 42 from + BPC Scan (2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane; C24H38O2Si2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	70.63	70.63			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	69.19	69.19			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	67.48	67.48			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2		999678-47-5			70.63	70.63			W9N08.L

+ Scan (rt: 17.39-17.40 min) **Peak 43 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	69.23	69.23			W9N08.L
No	LibSearch	(Z)-Methyl 2-(1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2"'-...	C19H28O7S2				999698-32-9	65.93	65.93			W9N08.L
No	LibSearch	{Hexyl-(heptahydrooctasila-sesquioxane)}	C15H40O3Si4				0-00-0	60.52	60.52			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			69.23	69.23			W9N08.L

+ Scan (rt: 17.77-17.79 min) **Peak 44 from + BPC Scan (Ethyl ester of 6-methyl-1,3-dihydrofuro[3,4-c]pyridine-7-carboxylic acid; C11H13NO3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Ethyl ester of 6-methyl-1,3-dihydrofuro[3,4-c]pyridine-7-carboxylic acid	C11H13NO3				92757-50-1	70.35	70.35			W9N08.L
No	LibSearch	2-(2-Cyanoethyl)-3,3-diethyl-4- and 5-cyanoisoxazolidine	C11H17N3O				89902-93-2	62.82	62.82			W9N08.L
No	LibSearch	2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	C18H26O3				5466-77-3	62.31	62.31			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Ethyl ester of 6-methyl-1,3-dihydrofuro[3,4-c]pyridine-7-carboxylic acid	C11H13NO3		92757-50-1			70.35	70.35			W9N08.L

+ Scan (rt: 17.90-17.93 min) **Peak 45 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	90.08	90.08			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	74.02	74.02			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	65.72	65.72			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			90.08	90.08			W9N08.L

+ Scan (rt: 18.02-18.05 min) **Peak 46 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	68.96	68.96			W9N08.L
No	LibSearch	1-Phenyl-5,5-dimethyl-4,6-dioxa-5-sila-8-nitrooct-1-ene	C13H19NO4Si				999405-61-6	57.63	57.63			W9N08.L
No	LibSearch	(E)-1-(tert-Butyldimethylsilyl)-2-decyl-1,4-pentadien-3-ol	C21H42OSi				999550-61-4	56.51	56.51			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			68.96	68.96			W9N08.L

+ Scan (rt: 18.18-18.21 min) **Peak 47 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	70.36	70.36			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	69.86	69.86			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	68.19	68.19			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			70.36	70.36			W9N08.L

+ Scan (rt: 18.41-18.42 min) **Peak 48 from + BPC Scan (3-(2',4'-DIMETHOXY-6'-PROPYLBENZOYLOXY)-2-HYDROXY-4-METHOXY-6-PROPYLBENOIC ACID; C23H28O8)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	3-(2',4'-DIMETHOXY-6'-PROPYLBENZOYLOXY)-2-HYDROXY-4-METHOXY-6-PROPYLBENOIC ACID	C23H28O8				69563-42-4	68.67	68.67			W9N08.L
No	LibSearch	4-(2',4'-dimethoxy-6'-propylbenzoyloxy)-2-hydroxy-6-pentylbenzoic acid	C24H30O7				104307-58-6	67.81	67.81			W9N08.L
No	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	63.57	63.57			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	3-(2',4'-DIMETHOXY-6'-PROPYLBENZOYLOXY)-2-HYDROXY-4-METHOXY-6-PROPYLBENOIC ACID	C23H28O8		69563-42-4			68.67	68.67			W9N08.L

+ Scan (rt: 18.45-18.48 min) **Peak 49 from + BPC Scan ((3R)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one; C14H11NO)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(3R)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C14H11NO				999205-14-4	63.37	63.37			W9N08.L
No	LibSearch	(3S)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C14H11NO				999205-14-5	63.28	63.28			W9N08.L
No	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	63.06	63.06			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(3R)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C14H11NO		999205-14-4			63.37	63.37			W9N08.L

+ Scan (rt: 18.50-18.52 min) **Peak 50 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.61	71.61			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	70.25	70.25			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	66.58	66.58			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			71.61	71.61			W9N08.L

+ Scan (rt: 18.66-18.69 min) **Peak 51 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	78.75	78.75			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	65.03	65.03			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	64.02	64.02			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			78.75	78.75			W9N08.L

+ Scan (rt: 18.70-18.72 min) **Peak 52 from + BPC Scan (2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane; C24H38O2Si2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	84.63	84.63			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	82.13	82.13			W9N08.L
No	LibSearch	(Z)-Methyl 2-(1'-[2"-(2"',2"'-Dimethoxyethyl)-1",3"-dithian-2"-yl]-2'-(2"'-...	C19H28O7S2				999698-32-9	77.95	77.95			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2		999678-47-5			84.63	84.63			W9N08.L

+ Scan (rt: 18.74-18.75 min) **Peak 53 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.23	71.23			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	67.24	67.24			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	66.29	66.29			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			71.23	71.23			W9N08.L

+ Scan (rt: 18.76-18.81 min) **Peak 54 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	84.22	84.22			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	72.69	72.69			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.20	72.20			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			84.22	84.22			W9N08.L

+ Scan (rt: 19.14-19.16 min) **Peak 55 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	88.37	88.37			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.46	73.46			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	66.93	66.93			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			88.37	88.37			W9N08.L

+ Scan (rt: 19.45-19.46 min) **Peak 56 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.28	72.28			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	69.41	69.41			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.89	67.89			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			72.28	72.28			W9N08.L

+ Scan (rt: 19.48-19.51 min) **Peak 57 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	85.23	85.23			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.55	72.55			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	71.42	71.42			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			85.23	85.23			W9N08.L

+ Scan (rt: 19.55-19.57 min) **Peak 58 from + BPC Scan**

+ Scan (rt: 19.61-19.62 min) **Peak 59 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	86.93	86.93			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.75	72.75			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	68.45	68.45			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			86.93	86.93			W9N08.L

+ Scan (rt: 19.79-19.80 min) **Peak 60 from + BPC Scan**

+ Scan (rt: 19.84-19.86 min) **Peak 61 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	88.65	88.65			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	74.04	74.04			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.43	67.43			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			88.65	88.65			W9N08.L

+ Scan (rt: 20.00-20.07 min) **Peak 62 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	71.74	71.74			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	70.39	70.39			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	69.84	69.84			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			71.74	71.74			W9N08.L

+ Scan (rt: 20.10-20.12 min) **Peak 63 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.32	72.32			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.05	67.05			W9N08.L
No	LibSearch	(Hexyl-(heptahydrooctasila-sesquioxane)]	C15H40O3Si4				0-00-0	63.26	63.26			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			72.32	72.32			W9N08.L

+ Scan (rt: 20.13-20.16 min) **Peak 64 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	86.21	86.21			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.41	71.41			W9N08.L
No	LibSearch	(Hexyl-(heptahydrooctasila-sesquioxane)]	C15H40O3Si4				0-00-0	62.49	62.49			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			86.21	86.21			W9N08.L

+ Scan (rt: 20.20-20.21 min) **Peak 65 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	87.28	87.28			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.12	73.12			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	68.49	68.49			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			87.28	87.28			W9N08.L

+ Scan (rt: 20.33-20.38 min) **Peak 66 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	85.58	85.58			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.41	71.41			W9N08.L
No	LibSearch	(Hexyl-(heptahydrooctasila-sesquioxane)]	C15H40O3Si4				0-00-0	62.45	62.45			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			85.58	85.58			W9N08.L

+ Scan (rt: 20.46-20.47 min) **Peak 67 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	69.77	69.77			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	69.68	69.68			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	68.19	68.19			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			69.77	69.77			W9N08.L

+ Scan (rt: 20.55-20.58 min) **Peak 68 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	82.32	82.32			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	69.11	69.11			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	67.39	67.39			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			82.32	82.32			W9N08.L

+ Scan (rt: 20.63-20.67 min) **Peak 69 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	85.61	85.61			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.95	72.95			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	71.46	71.46			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			85.61	85.61			W9N08.L

+ Scan (rt: 20.69-20.74 min) **Peak 70 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	82.24	82.24			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	68.49	68.49			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	67.36	67.36			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			82.24	82.24			W9N08.L

+ Scan (rt: 20.76-20.77 min) **Peak 71 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	88.36	88.36			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.89	73.89			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.75	67.75			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			88.36	88.36			W9N08.L

+ Scan (rt: 20.79-20.80 min) **Peak 72 from + BPC Scan (1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one; C16H13NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	85.36	85.36			W9N08.L
No	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	68.34	68.34			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2		116705-58-9			85.36	85.36			W9N08.L

+ Scan (rt: 20.85-20.86 min) **Peak 73 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	70.50	70.50			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	69.27	69.27			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	68.72	68.72			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			70.50	70.50			W9N08.L

+ Scan (rt: 20.88-20.90 min) **Peak 74 from + BPC Scan (1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one; C16H13NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	85.43	85.43			W9N08.L
No	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	67.74	67.74			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2		116705-58-9			85.43	85.43			W9N08.L

+ Scan (rt: 20.92-20.93 min) **Peak 75 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	87.65	87.65			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.07	73.07			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.63	67.63			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			87.65	87.65			W9N08.L

+ Scan (rt: 20.98-20.99 min) **Peak 76 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	71.02	71.02			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	69.50	69.50			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	69.30	69.30			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			71.02	71.02			W9N08.L

+ Scan (rt: 21.05-21.08 min) **Peak 77 from + BPC Scan (1-Phenyl-5,5-dimethyl-4,6-dioxa-5-sila-8-nitrooct-1-ene; C13H19NO4Si)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1-Phenyl-5,5-dimethyl-4,6-dioxa-5-sila-8-nitrooct-1-ene	C13H19NO4Si				999405-61-6	70.80	70.80			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	69.96	69.96			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	66.04	66.04			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1-Phenyl-5,5-dimethyl-4,6-dioxa-5-sila-8-nitrooct-1-ene	C13H19NO4Si		999405-61-6			70.80	70.80			W9N08.L

+ Scan (rt: 21.11-21.14 min) **Peak 78 from + BPC Scan (1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one; C16H13NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	85.39	85.39			W9N08.L
No	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	66.47	66.47			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2		116705-58-9			85.39	85.39			W9N08.L

+ Scan (rt: 21.15-21.17 min) **Peak 79 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.63	72.63			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	66.34	66.34			W9N08.L
No	LibSearch	(Hexyl-(heptahydrooctasilasesquioxane)]	C15H40O3Si4				0-00-0	63.56	63.56			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			72.63	72.63			W9N08.L

+ Scan (rt: 21.18-21.19 min) **Peak 80 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	69.35	69.35			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	63.89	63.89			W9N08.L
No	LibSearch	1,1,1,3,3,5,5-Heptamethyltrisiloxane	C7H22O2Si3				999238-34-3	61.67	61.67			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			69.35	69.35			W9N08.L

+ Scan (rt: 21.23-21.24 min) **Peak 81 from + BPC Scan ((S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one; C20H28O3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	69.20	69.20			W9N08.L
No	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	68.79	68.79			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	67.07	67.07			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3		999499-61-2			69.20	69.20			W9N08.L

+ Scan (rt: 21.39-21.40 min) **Peak 82 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	69.23	69.23			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	68.85	68.85			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	67.56	67.56			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			69.23	69.23			W9N08.L

+ Scan (rt: 21.43-21.47 min) **Peak 83 from + BPC Scan (2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane; C24H38O2Si2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	75.25	75.25			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	70.28	70.28			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	69.85	69.85			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2		999678-47-5			75.25	75.25			W9N08.L

+ Scan (rt: 21.55-21.56 min) **Peak 84 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	69.86	69.86			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	68.76	68.76			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	68.26	68.26			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			69.86	69.86			W9N08.L

+ Scan (rt: 21.63-21.64 min) **Peak 85 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	71.94	71.94			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	70.53	70.53			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	70.04	70.04			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			71.94	71.94			W9N08.L

+ Scan (rt: 21.67-21.69 min) **Peak 86 from + BPC Scan (2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane; C24H38O2Si2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	73.72	73.72			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.56	71.56			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	70.27	70.27			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2		999678-47-5			73.72	73.72			W9N08.L

+ Scan (rt: 21.71-21.73 min) **Peak 87 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	72.09	72.09			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	70.45	70.45			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	70.23	70.23			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			72.09	72.09			W9N08.L

+ Scan (rt: 21.74-21.76 min) **Peak 88 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	83.73	83.73			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	81.75	81.75			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	81.56	81.56			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			83.73	83.73			W9N08.L

+ Scan (rt: 21.81-21.83 min) **Peak 89 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	73.98	73.98			W9N08.L
No	LibSearch	2-(1-Methyl-1H-2-pyrroly)quinoline	C14H12N2				999203-02-0	72.28	72.28			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	72.22	72.22			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			73.98	73.98			W9N08.L

+ Scan (rt: 21.84-21.86 min) **Peak 90 from + BPC Scan (1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one; C16H13NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	85.42	85.42			W9N08.L
No	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	67.82	67.82			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2		116705-58-9			85.42	85.42			W9N08.L

+ Scan (rt: 21.88-21.89 min) **Peak 91 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	69.69	69.69			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	69.65	69.65			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	68.16	68.16			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			69.69	69.69			W9N08.L

+ Scan (rt: 21.94-21.96 min) **Peak 92 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	72.89	72.89			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	71.05	71.05			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	70.94	70.94			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			72.89	72.89			W9N08.L

+ Scan (rt: 21.98-22.01 min) **Peak 93 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	71.51	71.51			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	69.91	69.91			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	69.66	69.66			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			71.51	71.51			W9N08.L

+ Scan (rt: 22.08-22.09 min) **Peak 94 from + BPC Scan ((S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one; C20H28O3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	69.14	69.14			W9N08.L
No	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	68.21	68.21			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	68.16	68.16			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3		999499-61-2			69.14	69.14			W9N08.L

+ Scan (rt: 22.17-22.18 min) **Peak 95 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	86.86	86.86			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.79	72.79			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	68.69	68.69			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			86.86	86.86			W9N08.L

+ Scan (rt: 22.19-22.21 min) **Peak 96 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	86.49	86.49			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.08	73.08			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	69.99	69.99			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			86.49	86.49			W9N08.L

+ Scan (rt: 22.35-22.37 min) **Peak 97 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.09	72.09			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	71.65	71.65			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	69.75	69.75			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			72.09	72.09			W9N08.L

+ Scan (rt: 22.38-22.40 min) **Peak 98 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	73.26	73.26			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	71.79	71.79			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	71.34	71.34			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			73.26	73.26			W9N08.L

+ Scan (rt: 22.58-22.60 min) **Peak 99 from + BPC Scan (3-(2',4'-DIMETHOXY-6'-PROPYLBENZOYLOXY)-2-HYDROXY-4-METHOXY-6-PROPYLBENOIC ACID; C23H28O8)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	3-(2',4'-DIMETHOXY-6'-PROPYLBENZOYLOXY)-2-HYDROXY-4-METHOXY-6-PROPYLBENOIC ACID	C23H28O8				69563-42-4	68.31	68.31			W9N08.L
No	LibSearch	4-(2',4'-dimethoxy-6'-propylbenzoyloxy)-2-hydroxy-6-pentylbenzoic acid	C24H30O7				104307-58-6	67.75	67.75			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	63.88	63.88			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	3-(2',4'-DIMETHOXY-6'-PROPYLBENZOYLOXY)-2-HYDROXY-4-METHOXY-6-PROPYLBENOIC ACID	C23H28O8		69563-42-4			68.31	68.31			W9N08.L

+ Scan (rt: 22.63-22.64 min) **Peak 100 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	88.66	88.66			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.37	73.37			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	66.07	66.07			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			88.66	88.66			W9N08.L

+ Scan (rt: 22.70-22.72 min) **Peak 101 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	72.21	72.21			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	70.44	70.44			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	70.37	70.37			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			72.21	72.21			W9N08.L

+ Scan (rt: 22.77-22.79 min) **Peak 102 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.39	71.39			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	67.81	67.81			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	64.39	64.39			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			71.39	71.39			W9N08.L

+ Scan (rt: 22.85-22.89 min) **Peak 103 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	89.14	89.14			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.63	73.63			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	65.57	65.57			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			89.14	89.14			W9N08.L

+ Scan (rt: 22.93-22.97 min) **Peak 104 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	86.24	86.24			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.07	73.07			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	70.45	70.45			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			86.24	86.24			W9N08.L

+ Scan (rt: 22.98-22.99 min) **Peak 105 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.39	71.39			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	65.72	65.72			W9N08.L
No	LibSearch	(Hexyl-(heptahydrooctasila-sesquioxane)]	C15H40O3Si4				0-00-0	62.48	62.48			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			71.39	71.39			W9N08.L

+ Scan (rt: 23.00-23.01 min) **Peak 106 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.36	72.36			W9N08.L
No	LibSearch	2,3-bis(trimethylsiloxy)-2,3-bis(4'-methylphenyl)butane	C24H38O2Si2				999678-47-5	69.32	69.32			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	66.93	66.93			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			72.36	72.36			W9N08.L

+ Scan (rt: 23.08-23.09 min) **Peak 107 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	89.50	89.50			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.57	73.57			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	64.59	64.59			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			89.50	89.50			W9N08.L

+ Scan (rt: 23.11-23.13 min) **Peak 108 from + BPC Scan (7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol; C22H36O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	71.64	71.64			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	70.51	70.51			W9N08.L
No	LibSearch	(Hexyl-(heptahydrooctasilasesquioxane)]	C15H40O3Si4				0-00-0	62.51	62.51			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6		999654-24-5			71.64	71.64			W9N08.L

+ Scan (rt: 23.15-23.17 min) **Peak 109 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	87.78	87.78			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.13	73.13			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.49	67.49			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			87.78	87.78			W9N08.L

+ Scan (rt: 23.22-23.26 min) **Peak 110 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	88.30	88.30			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.43	73.43			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.00	67.00			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			88.30	88.30			W9N08.L

+ Scan (rt: 23.28-23.32 min) **Peak 111 from + BPC Scan (1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one; C16H13NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	85.39	85.39			W9N08.L
No	LibSearch	3-[o-Methoxyphenyl]-5,6-[(1',2'-cyclohexyl)dihydro]thiazolo[2,3-c]-s-triazole	C15H17N3OS				999422-75-2	68.15	68.15			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2		116705-58-9			85.39	85.39			W9N08.L

+ Scan (rt: 23.34-23.36 min) **Peak 112 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	85.66	85.66			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.50	72.50			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	70.46	70.46			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			85.66	85.66			W9N08.L

+ Scan (rt: 23.41-23.42 min) **Peak 113 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	86.54	86.54			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.65	72.65			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	69.02	69.02			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			86.54	86.54			W9N08.L

+ Scan (rt: 23.46-23.46 min) **Peak 114 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	85.05	85.05			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	82.89	82.89			W9N08.L
No	LibSearch	quinuclidinium-methanesulfonate	C8H17NO3S				126821-96-3	82.72	82.72			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			85.05	85.05			W9N08.L

+ Scan (rt: 23.56-23.56 min) **Peak 115 from + BPC Scan (6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion; C12H15DNO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	84.78	84.78			W9N08.L
No	LibSearch	.alpha.-Fluoro-(p-methyl)chalcone	C16H13FO				999292-95-3	82.70	82.70			W9N08.L
No	LibSearch	2-(1-Methyl-1H-2-pyrrolyl)quinoline	C14H12N2				999203-02-0	82.16	82.16			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2		999196-11-0			84.78	84.78			W9N08.L

+ Scan (rt: 23.58-23.60 min) **Peak 116 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	86.86	86.86			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.11	73.11			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	69.30	69.30			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			86.86	86.86			W9N08.L

+ Scan (rt: 23.84-23.85 min) **Peak 117 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	87.54	87.54			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.08	73.08			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.89	67.89			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			87.54	87.54			W9N08.L

+ Scan (rt: 24.01-24.01 min) **Peak 118 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	87.99	87.99			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	73.18	73.18			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	67.15	67.15			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			87.99	87.99			W9N08.L

+ Scan (rt: 24.17-24.18 min) **Peak 119 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	87.14	87.14			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.77	72.77			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	68.08	68.08			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			87.14	87.14			W9N08.L

+ Scan (rt: 24.23-24.25 min) **Peak 120 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	85.31	85.31			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	72.45	72.45			W9N08.L
No	LibSearch	1-(Pent-4-ynyl)pyrano[3,4-b]indol-3-one	C16H13NO2				116705-58-9	71.04	71.04			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			85.31	85.31			W9N08.L

+ Scan (rt: 24.26-24.28 min) **Peak 121 from + BPC Scan (Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...; C21H26O6)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6				999620-34-3	69.06	69.06			W9N08.L
No	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	66.94	66.94			W9N08.L
No	LibSearch	(3R)-3-Phenyl-2,3-dihydro-1H-isoindol-1-one	C14H11NO				999205-14-4	64.28	64.28			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Phenyl 4-[bis(ethoxycarbonyl)but-3-ynyl]-2,3,4-trideoxy-.alpha.,L-glcero-pen...	C21H26O6		999620-34-3			69.06	69.06			W9N08.L

+ Scan (rt: 24.47-24.49 min) **Peak 122 from + BPC Scan ((S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one; C20H28O3)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3				999499-61-2	68.52	68.52			W9N08.L
No	LibSearch	6,7-Dimethoxy-2-methyl-3,4-dihydro[1-D]isoquinolinium ion	C12H15DNO2				999196-11-0	67.96	67.96			W9N08.L
No	LibSearch	7,9-(p-Methoxyphenylidenedioxy)-5-methoxy-2,4,6,8-tetraamethylnonan-1,3-diol	C22H36O6				999654-24-5	67.75	67.75			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-dodecen-1-one	C20H28O3		999499-61-2			68.52	68.52			W9N08.L

MassHunter Qual 10.0
(End of Report)

U trećem uzorku ispitivane su ampule za poticanje rasta kose kod žena. Na deklaraciji kao aktivne tvari koje potiču rast kose naznačene su aminexil, arginin, protein sp94, vitamin b6, niacinamid te oktein. Analizom je utvrđeno prisustvo samo piroktona, kofeina, oktadekatriena i niacinamida te nisu pronađeni nikakvi drugi kao niti toksični sastojci.

Slijede grafički prikazani rezultati trećeg uzorka.

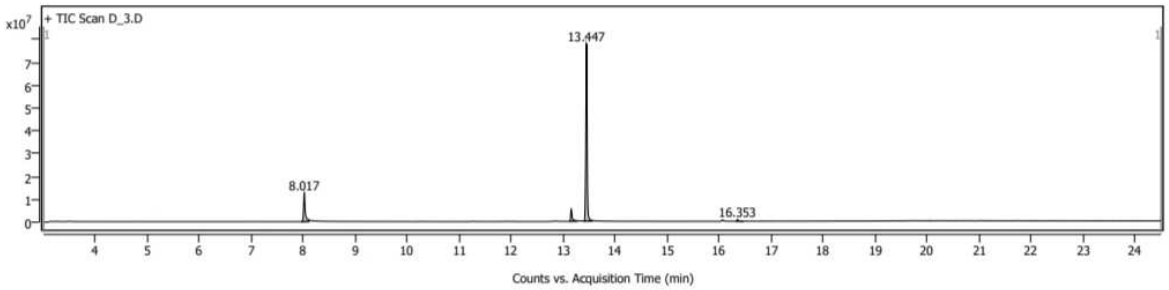
Analysis Report

Agilent Technologies

Sample Information

Name	3	**Data File Path**	D:\MassHunter\GCMS\1\data\Davorka\D_3.D
Sample ID		**Acq. Time (Local)**	7/27/2021 12:12:33 PM (UTC+02:00)
Instrument	KTF_GCMS_QQQ	**Method Path (Acq)**	D:\MassHunter\GCMS\1\methods\Davorka_1M.M
MS Type	QQQ	**Version (Acq SW)**	MassHunter GC/MS Acquisition 10.0.368 14-Feb-2019 Copyright © 1989-2018 Agilent Technologies, Inc.
Inj. Vol. (ul)	1	**IRM Status**	
Position	3	**Method Path (DA)**	D:\MassHunter\Methods\10.0\IZVJESTAJ.m
Plate Pos.		**Target Source Path**	
Operator	Davorka	**Result Summary**	

Sample Chromatograms



Chromatogram Peaks

Peak	Start	RT	End	Height	Area	Area %	SNR
1	7.965	8.017	8.103	12595433	27970790	15.30	
2	13.123	13.154	13.261	5253445	11140665	6.09	
3	13.402	13.447	13.554	77782288	141963746	77.63	
4	16.316	16.353	16.457	782961	1786106	0.98	

Sample Spectra

+ Scan (rt: 7.99-8.07 min) **Peak 1 from + TIC Scan (3-Pyridinecarboxamide; C6H6N2O)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	3-Pyridinecarboxamide	C6H6N2O				98-92-0	96.02	96.02			W9N08.L
No	LibSearch	3-Pyridinecarboxamide	C6H6N2O				98-92-0	95.14	95.14			W9N08.L
No	LibSearch	Niacinamide	C6H6N2O				98-92-0	94.77	94.77			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	3-Pyridinecarboxamide	C6H6N2O		98-92-0			96.02	96.02			W9N08.L

+ Scan (rt: 13.13-13.20 min) **Peak 2 from + TIC Scan (Piroctone ; C14H23NO2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Piroctone	C14H23NO2				50650-76-5	79.54	79.54			W9N08.L
No	LibSearch	1-Allyl (4-Methoxyphenyl) sulfide	C10H12OS				999129-46-0	61.44	61.44			W9N08.L
No	LibSearch	Piroctone	C14H23NO2				50650-76-5	59.56	59.56			NIST17.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Piroctone	C14H23NO2		50650-76-5			79.54	79.54			W9N08.L

+ Scan (rt: 13.42-13.47 min) **Peak 3 from + TIC Scan (Caffeine; C8H10N4O2)**

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	Caffeine	C8H10N4O2				58-08-2	96.50	96.50			W9N08.L
No	LibSearch	Caffeine	C8H10N4O2				58-08-2	95.08	95.08			W9N08.L
No	LibSearch	Caffeine	C8H10N4O2				58-08-2	95.04	95.04			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	Caffeine	C8H10N4O2		58-08-2			96.50	96.50			W9N08.L

+ Scan (rt: 16.33-16.42 min) **Peak 4 from + TIC Scan (1,E-11,Z-13-Octadecatriene ; C18H32)**

Slika 11.

Analysis Report

Agilent | Trusted Answ

Spectrum Identification Table

Best	ID Source	Name	Formula	Species	m/z	Diff (ppm)	CAS	Score	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
Yes	LibSearch	1,E-11,Z-13-Octadecatriene	C18H32				80625-36-1	75.06	75.06			W9N08.L
No	LibSearch	Z,E-7,11-Hexadecadien-1-yl acetate	C18H32O2				51607-94-4	73.97	73.97			W9N08.L
No	LibSearch	9,12-Octadecadien-1-ol, (Z,Z)-	C18H34O				506-43-4	73.93	73.93			W9N08.L

Best	Name	Formula	m/z (prec.)	CAS	RT (DB)	RT Diff	Score	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
Yes	1,E-11,Z-13-Octadecatriene	C18H32		80625-36-1			75.06	75.06			W9N08.L

MassHunter Qual 10.0
(End of Report)

5. RASPRAVA

Ovo istraživanje je obuhvatilo isključivo kvalitativnu analizu te je u donošenju zaključka nužna kvantitativna analiza kao i primjena drugih instrumentalnih tehnika odnosno drugačiji načini pripreme uzorka.

Pronađene tvari su u tragovima stoga svaka interpretacija zahtjeva ozbiljan pristup kako se ne bi donijeli krivi zaključci. Velik broj populacije nije upućen u točnu interpretaciju rezultata pa bi na samu pomisao određenih tvari mogli donijeti krivi zaključak što rezultira štetnim učinkom, a zapravo se radi o beznačajnim tragovima koji predstavljaju šum instrumenta jer se radi o vrlo visokoj osjetljivosti. Program za usporedbu daje popis svih eventualnih podudaranja, a stvar je analitičara da je podesi na prihvatljivu razinu te time izbjegne krive zaključke. Stoga rezultat prikazan za uzorak pod br. 1 ne predstavlja stvarni rezultat već upravo popis artefakata u analizi.

Prilikom analize prvog uzorka u kojem se nalazila otopina za vlasište pronađen je oxiran ili etilen oksid. Koristi se u proizvodnji tenzida te kao sterilizator za zdravstvene materijale te druge proizvode osjetljive na toplinu. Kroz kožu se može apsorbirati iz plinske faze ili vodenih otopina te se ravnomjerno rasporedi po cijelom tijelu. Istraživanja na životinjama pokazuju da izaziva mutaciju gena, prilikom testiranja in vivo te in vitro. Toksičan je sastojak koji može dovesti do iritacija te ima potencijalno štetan učinak na ljudsko zdravlje. (42)

Pronađeni spojevi karbamata su esteri karbaminske kiseline koji se obično koriste kao insekticidi. N-metilkarbamatni insekticidi proizvode svoju toksičnost inhibiranjem enzima acetilkolinesteraze, a niske su toksičnosti za sisavce. (43)

Katinon je prirodni analog beta-ketona amfetamina koji se nalazi u lišću biljke Catha edulis, a sintetički katinoni su derivati ovog spoja. (44) Pripada loše reguliranoj skupini spojeva koji dovode do povećanja budnosti, uzbuđenja i uznemirenosti. Djeluju različitim mehanizmima, ali ne izravnom pobudom neurona. (45) Izloženost i upotreba sintetskih katinona postaju sve češći unatoč nedostatku znanstvnih istraživanja i razumijevanja moguće štetnosti tvari. (44) Nema znanstvenih dokaza kojim bi se ovaj sastojak povezao s poticanjem rasta kose

te tako opravdao svoju ulogu u otopini stoga smtramo da je i ovaj trag rezultat prevelike osjetljivosti i spada u artefakte.

Veliko iznenađenje među pronađenim sastojcima izazvao je rimantadin. Radi se o cikličkom aminu i alfa-metil derivatu amantadina s antivirusnim djelovanjem. Iako se ne razumije točan mehanizam djelovanja rimantadina, čini se da ovo sredstvo ispoljava svoj antivirusni učinak protiv virusa influence A ometajući funkciju transmembranske domene virusnog M2 proteina, čime se sprječava omatanje virusa i kasnije oslobađanje zarazne virusne nukleinske kiseline u citoplazmu inficiranih stanica. (46) Nema poveznice između rimantadina i poticanja rasta kose stoga kao i prethodno opisana tvar, smatramo da je i ovaj trag rezultat prevelike osjetljivosti i spada u artefakte.

Među pronađenim spojevima toksičan je i fluoracetamid primarno zbog kemijskih reakcija kojima se prevodi u fluoroacetat. Fluoroacetat je spoj koji toksičnost ispoljava tako da sprječava ciklus limunske kiseline. Srce i središnji živčani sustav su najkritičnija tkiva kada se radi o inhibiciji metabolizma energije. (47)

Zaključno, u uzorku br. 1 pronađeno je mnoštvo tragova koje bi ukazale na njihovo nedozvoljeno i nepoželjno prisustvo, međutim smatramo da su svi i tragovi ipak samo artefakti te da ispitivan uzorak ne sadžava takve toksične tvari.

U trećem analiziranom uzorku nismo dokazali značajno prisustvo toksičnih tvari osim visokog signala kofeina što predstavlja visoku koncentraciju.

U trećem ispitivanom uzorku među pronađenim spojevima kofein i niacinamid imaju opravdanu ulogu u spomenutim ampulama međutim nemaju potporu ostalih navedenih aktivnih sastojaka za potpuni učinak koji je obećan kupnjom proizvoda. Pirokton se nalazi među pomoćnim tvarima na deklaraciji te je pronađen ovom analizom. Ne može se povezati izravno s poticanjem rasta kose nego ima ulogu antimikrobne komponente. Pregledom baze podataka nije utvrđena toksičnost piroktona. (48) Kofein je stimulans koji pomaže u poticanju rasta kose međutim postavlja se pitanje zašto se nalazi u punoj većoj količini u odnosu na druge sastojke.

6. ZAKLJUČCI

1.U prvom uzorku pronašli smo više tvari nego što je registrirano na samom proizvodu međutim one su rezultat visokog praga osjetljivost.

2. Naše istraživanje je obuhvatilo samo kvalitativnu analizu , a za potpuno razumijevanje rezultata neophodno je napraviti i kvantitativnu analizu.

3. U trećem uzorku nismo pronašli sve tvari navedene na deklaraciji.

4. U trećem uzorku nismo pronašli obilježje kojem bi opravdali naziv ampula za žene.

5. Detaljna interpretacija rezultata zahtjeva puno znanja te dodatnih analiza kako se ne bi donijeli krivi zaključci s obzirom na dobivene rezultate.

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8. SAŽETAK

Naslov rada:

Preparati protiv ispadanja kose: sastav i mogući utjecaj na zdravlje

Ciljevi:

Kvalitativnom metodom (GC-MS) odrediti sastav preparata protiv ispadanja kose te usporediti navode deklaracija s dobivenim rezultatima.

Materijali i metode:

Ispitana su 2 uzorka preparata protiv ispadanja kose. Za pripremu uzorka korištene su staklene Petrijeve zdjelice na koje je nanesen uzorak volumena 100 µL. Uzorci su ekstrahirani smjesom organskih otapala, kloroforma, etil acetata i N-heksana u jednakom omjeru (v/v/v= 1:1:1), te su potom postavljeni u digestor na sušenje u struji zraka. Kromatografska analiza pripremljenih ekstrakata izvedena je na plinskom kromatografu sa spektrometrom masa, metodom koja omogućava istovremeno snimanje ukupnog ionskog kromatograma (*engl. Total ion chromatogram*, TIC) u području od 40 – 600 m/z i snimanje samo odabranih iona (*engl. Single ion monitoring*, SIM).

Rezultati:

Kvalitativnom analizom uzoraka dobili smo rezultate koji su izlistani u analitičkom izvješću. U prvom uzorku su pronađene tvari koje nisu navedene među pomoćnim tvarima, ali prema visini signala možemo zaključiti da se radi o tvarima koje se nalaze u tragovima. U trećem uzorku nismo pronašli sve tvari koje proizvođač navodi na ambalaži, a kofein koji je jedan od sastojaka je pokazao jako visok signal što odgovara visokoj koncentraciji.

Zaključak:

Ovim istraživanjem je provedena samo kvalitativna analiza te bi za detaljniju obradu dobivenih podataka trebalo provesti i kvantitativnu analizu kako bi u potpunosti točno interpretirali rezultate.

9. SUMMARY

Diploma thesis title:

Anti-hair loss products : compositions and possible health impact

Objectives:

Qualitative determination of ingredients in products for hair loss using GC-MS method,as well as the comparison of the results with those declared on the product.

Material and methods:

Two samples of anti-hair loss products were tested. Petri dishes were used to prepare the sample and volume of 100 μL was applied. Samples were extraced with a mixture of organic solvents, chloroform, ethyl acetate and N-hexane in equal ratio (v / v / v = 1: 1: 1), and then placed in a digester to air dry. Chromatographic analysis of the prepared extracts was performed on a gas chromatograph with a mass spectrometer, a method that allows simultaneous recording of the total ion chromatogram (TIC) in the range of 40 - 600 m / z and recording only selected ions (single ion monitoring, SIM).

Results:

By qualitative analysis of the samples, we obtained the results listed in the analytical report. In the first sample, substances were found that are not listed among the excipients, but according to the signal height, we can conclude that these are trace substances. In the third sample, we did not find all the substances listed by the manufacturer on the packaging, and caffeine, which is one of the ingredients, showed a very high signal, which corresponds to a high concentration.

Conclusion:

With this research, only a qualitative analysis was performed, and for a more detailed processing of the obtained data, a quantitative analysis should be performed in order to fully interpret the results.

10. ŽIVOTOPIS

Ime i prezime: Ines Jović

Datum rođenja: 11.04.1997.

Mjesto rođenja: Zadar, Republika Hrvatska

Obrazovanje:

- Osnovna škola Šimuna Kožičića Benje, Zadar
- Srednja škola Jurja Barakovića, Zadar
- Integrirani studij: Farmacija, Medicinski fakultet u Splitu
- Stručno osposobljavanje: 6 mjeseci u ljekarničkoj jedinici SDŽ „ Trstenik “

Dodatne aktivnosti:

- Članica Hrvatske udruge studenata farmacije i medicinske biokemije - CPSA